



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:28 am GMT

PDB ID : 1DCU
Title : REDOX SIGNALING IN THE CHLOROPLAST: STRUCTURE OF OXIDIZED PEA FRUCTOSE-1,6-BISPHOSPHATE PHOSPHATASE
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Deposited on : 1999-11-05
Resolution : 2.20 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

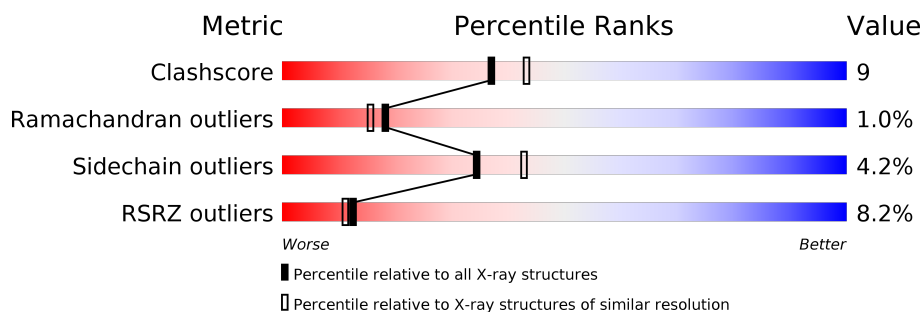
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	357	<div> <div>9%</div> <div> <div></div> <div>62%</div> <div>24%</div> <div>7%</div> <div>8%</div> </div> </div>
1	B	357	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	357	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>24%</div> <div>• •</div> <div>8%</div> </div> </div>
1	D	357	<div> <div>10%</div> <div> <div></div> <div>68%</div> <div>18%</div> <div>• •</div> <div>9%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10102 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FRUCTOSE-1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2507	1590	408	499	10			
1	B	323	Total	C	N	O	S	0	0	0
			2449	1558	401	480	10			
1	C	328	Total	C	N	O	S	0	0	0
			2497	1586	411	490	10			
1	D	325	Total	C	N	O	S	0	0	0
			2454	1561	402	481	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ALA	ILE	ENGINEERED	UNP P46275
B	103	ALA	ILE	ENGINEERED	UNP P46275
C	103	ALA	ILE	ENGINEERED	UNP P46275
D	103	ALA	ILE	ENGINEERED	UNP P46275
A	232	LYS	GLU	ENGINEERED	UNP P46275
B	232	LYS	GLU	ENGINEERED	UNP P46275
C	232	LYS	GLU	ENGINEERED	UNP P46275
D	232	LYS	GLU	ENGINEERED	UNP P46275

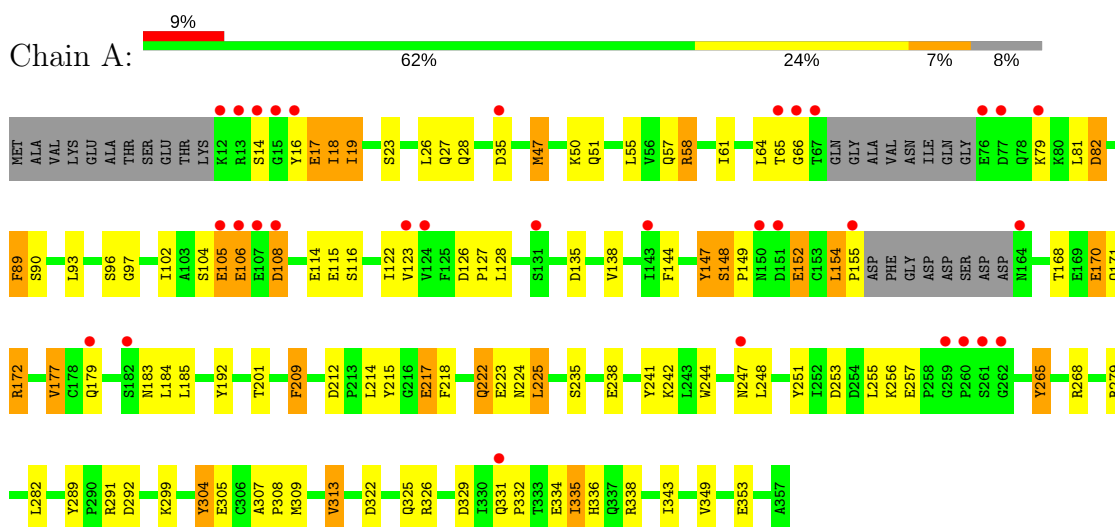
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		
2	B	56	Total	O	0	0
			56	56		
2	C	47	Total	O	0	0
			47	47		
2	D	52	Total	O	0	0
			52	52		

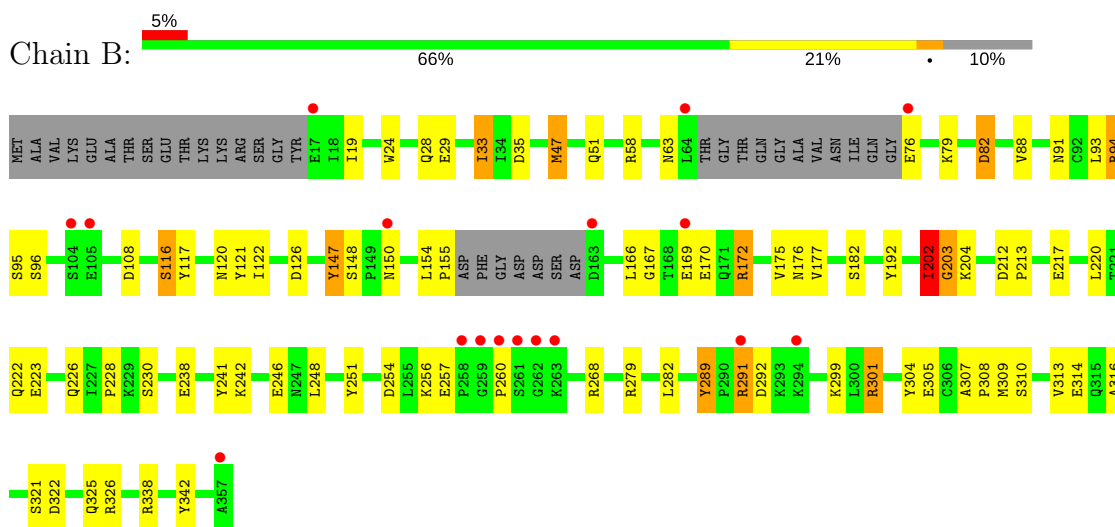
3 Residue-property plots [i](#)

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

• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE

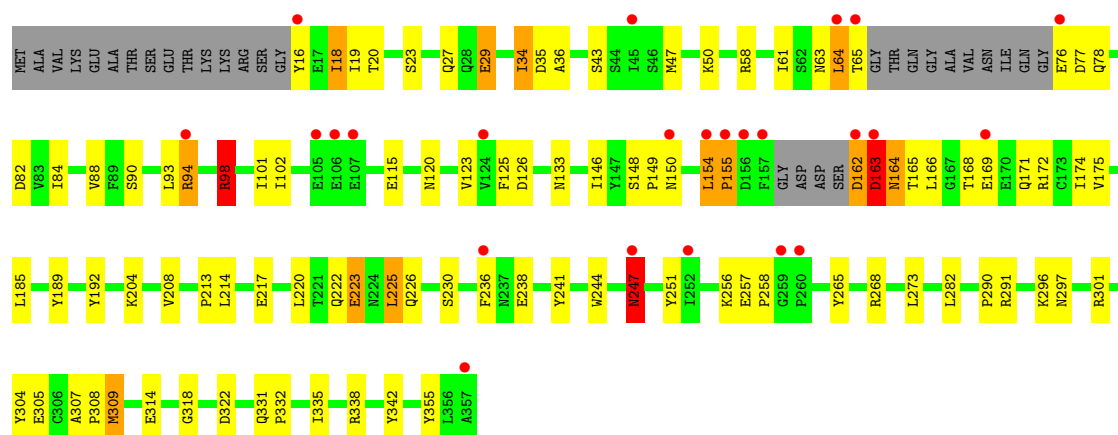


• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE

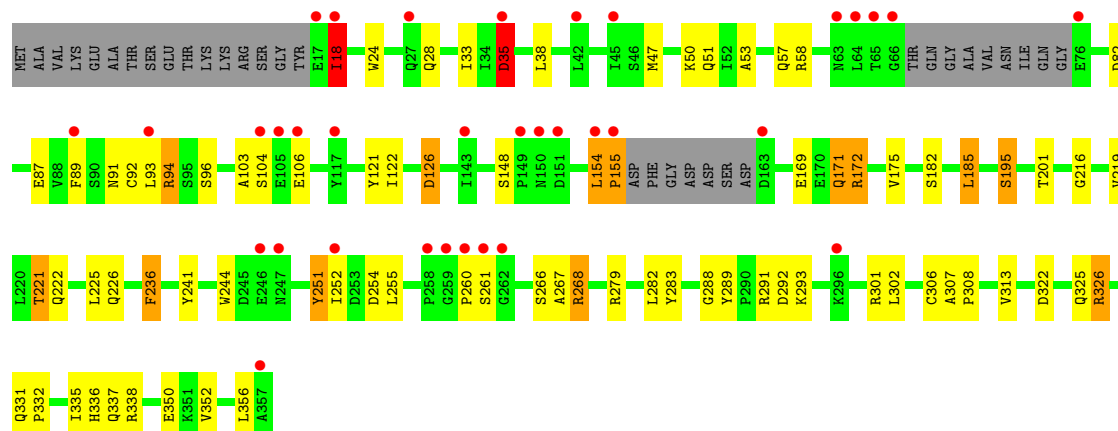


• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE





• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.60Å 126.32Å 78.02Å 90.00° 97.73° 90.00°	Depositor
Resolution (Å)	23.80 – 2.20 23.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (23.80-2.20) 99.6 (23.80-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.247 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10102	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.87	0/2553	1.92	63/3463 (1.8%)
1	B	1.01	3/2493 (0.1%)	1.97	63/3383 (1.9%)
1	C	0.92	0/2541	1.85	52/3444 (1.5%)
1	D	0.92	1/2499 (0.0%)	1.80	40/3393 (1.2%)
All	All	0.93	4/10086 (0.0%)	1.89	218/13683 (1.6%)

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	5
1	B	0	3
1	C	0	1
1	D	0	2
All	All	0	11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	ILE	C-O	7.30	1.37	1.23
1	D	195	SER	CA-CB	7.23	1.63	1.52
1	B	241	TYR	CE2-CZ	-5.06	1.31	1.38
1	B	230	SER	CB-OG	-5.03	1.35	1.42

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ILE	CA-C-N	21.39	158.98	116.20
1	C	162	ASP	C-N-CA	21.25	174.83	121.70
1	A	147	TYR	CB-CG-CD1	19.57	132.74	121.00
1	B	202	ILE	CA-C-O	-19.06	80.08	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ARG	NE-CZ-NH1	17.35	128.98	120.30
1	C	58	ARG	NE-CZ-NH2	-16.16	112.22	120.30
1	A	147	TYR	CB-CG-CD2	-16.13	111.32	121.00
1	D	94	ARG	NE-CZ-NH2	15.32	127.96	120.30
1	D	268	ARG	NE-CZ-NH2	15.14	127.87	120.30
1	B	94	ARG	NE-CZ-NH1	-14.62	112.99	120.30
1	D	279	ARG	NE-CZ-NH2	-14.14	113.23	120.30
1	B	94	ARG	NE-CZ-NH2	13.26	126.93	120.30
1	B	322	ASP	CB-CG-OD2	-12.51	107.05	118.30
1	B	301	ARG	NE-CZ-NH1	-12.38	114.11	120.30
1	B	268	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	A	253	ASP	CB-CG-OD1	12.31	129.38	118.30
1	B	202	ILE	C-N-CA	11.77	147.01	122.30
1	D	279	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	B	108	ASP	CB-CG-OD1	11.66	128.79	118.30
1	A	82	ASP	CB-CG-OD2	11.40	128.56	118.30
1	A	338	ARG	NE-CZ-NH2	-11.35	114.62	120.30
1	A	172	ARG	NE-CZ-NH1	-10.78	114.91	120.30
1	C	301	ARG	NE-CZ-NH1	-10.71	114.94	120.30
1	B	147	TYR	CB-CG-CD1	10.65	127.39	121.00
1	B	212	ASP	CB-CG-OD2	-10.61	108.75	118.30
1	C	98	ARG	CD-NE-CZ	10.57	138.41	123.60
1	A	212	ASP	CB-CG-OD2	10.56	127.80	118.30
1	A	279	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	B	202	ILE	N-CA-C	-10.00	84.00	111.00
1	D	338	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	B	241	TYR	CB-CG-CD2	9.56	126.74	121.00
1	B	326	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	C	172	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	D	236	PHE	CG-CD1-CE1	9.48	131.23	120.80
1	B	291	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	D	87	GLU	OE1-CD-OE2	-9.20	112.26	123.30
1	C	58	ARG	NH1-CZ-NH2	9.14	129.46	119.40
1	B	338	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	C	162	ASP	O-C-N	-9.00	108.30	122.70
1	D	104	SER	N-CA-CB	8.96	123.94	110.50
1	B	35	ASP	N-CA-CB	-8.93	94.53	110.60
1	A	251	TYR	CB-CG-CD2	-8.74	115.75	121.00
1	D	94	ARG	NE-CZ-NH1	-8.74	115.93	120.30
1	B	82	ASP	CB-CG-OD1	8.64	126.08	118.30
1	A	326	ARG	CD-NE-CZ	8.58	135.61	123.60
1	A	338	ARG	NH1-CZ-NH2	8.52	128.77	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	35	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	C	29	GLU	CA-CB-CG	8.51	132.13	113.40
1	C	322	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	C	82	ASP	CB-CG-OD2	8.43	125.89	118.30
1	D	254	ASP	CB-CG-OD1	8.37	125.83	118.30
1	A	279	ARG	CD-NE-CZ	8.22	135.10	123.60
1	A	58	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	D	338	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	D	82	ASP	CB-CG-OD1	8.06	125.56	118.30
1	D	103	ALA	N-CA-CB	-8.04	98.84	110.10
1	B	29	GLU	OE1-CD-OE2	-7.96	113.75	123.30
1	A	326	ARG	NH1-CZ-NH2	-7.59	111.05	119.40
1	A	329	ASP	CB-CG-OD1	7.43	124.99	118.30
1	A	338	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	B	212	ASP	CB-CG-OD1	7.36	124.92	118.30
1	C	162	ASP	CA-C-O	7.28	135.39	120.10
1	A	292	ASP	CB-CG-OD2	7.27	124.85	118.30
1	B	108	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	A	108	ASP	CA-CB-CG	7.26	129.37	113.40
1	A	152	GLU	N-CA-CB	-7.23	97.59	110.60
1	A	126	ASP	CB-CG-OD1	7.17	124.76	118.30
1	C	251	TYR	CB-CG-CD2	-7.17	116.70	121.00
1	A	265	TYR	CB-CG-CD2	-7.08	116.75	121.00
1	B	172	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	241	TYR	CB-CG-CD1	-7.08	116.75	121.00
1	C	29	GLU	OE1-CD-OE2	-7.05	114.84	123.30
1	B	192	TYR	CB-CG-CD1	-6.99	116.81	121.00
1	B	121	TYR	CB-CG-CD1	-6.99	116.81	121.00
1	C	58	ARG	CD-NE-CZ	-6.97	113.84	123.60
1	A	268	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	322	ASP	CB-CG-OD1	6.95	124.56	118.30
1	C	314	GLU	OE1-CD-OE2	-6.95	114.96	123.30
1	C	225	LEU	O-C-N	-6.89	111.67	122.70
1	B	126	ASP	CB-CG-OD2	-6.87	112.11	118.30
1	C	35	ASP	N-CA-CB	-6.86	98.25	110.60
1	C	155	PRO	N-CA-CB	6.84	111.51	103.30
1	A	170	GLU	OE1-CD-OE2	6.75	131.40	123.30
1	D	121	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	D	326	ARG	CD-NE-CZ	-6.72	114.19	123.60
1	B	291	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	35	ASP	CB-CA-C	-6.68	97.05	110.40
1	B	35	ASP	CB-CG-OD2	-6.65	112.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	C	338	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	36	ALA	CB-CA-C	-6.58	100.22	110.10
1	D	292	ASP	CB-CG-OD1	6.57	124.22	118.30
1	A	58	ARG	NH1-CZ-NH2	6.57	126.63	119.40
1	B	120	ASN	CA-CB-CG	-6.56	98.97	113.40
1	C	338	ARG	CD-NE-CZ	6.55	132.77	123.60
1	C	304	TYR	CB-CG-CD2	6.54	124.92	121.00
1	B	301	ARG	NH1-CZ-NH2	6.52	126.58	119.40
1	B	222	GLN	CB-CG-CD	6.51	128.52	111.60
1	C	125	PHE	CB-CG-CD2	6.51	125.35	120.80
1	A	89	PHE	CB-CG-CD2	6.47	125.33	120.80
1	C	163	ASP	N-CA-C	-6.47	93.54	111.00
1	B	192	TYR	CB-CG-CD2	6.45	124.87	121.00
1	B	126	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	58	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	B	182	SER	CB-CA-C	6.41	122.28	110.10
1	B	326	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
1	D	251	TYR	CB-CG-CD1	-6.36	117.19	121.00
1	A	225	LEU	O-C-N	-6.36	112.53	122.70
1	B	117	TYR	C-N-CA	6.33	137.53	121.70
1	B	305	GLU	OE1-CD-OE2	-6.32	115.72	123.30
1	C	251	TYR	CB-CG-CD1	6.31	124.78	121.00
1	C	98	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	201	THR	CA-CB-CG2	6.30	121.22	112.40
1	D	195	SER	CA-CB-OG	-6.30	94.19	111.20
1	B	292	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	A	309	MET	CA-CB-CG	6.29	123.99	113.30
1	B	58	ARG	CD-NE-CZ	-6.25	114.84	123.60
1	A	82	ASP	OD1-CG-OD2	-6.21	111.51	123.30
1	D	172	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	135	ASP	CB-CG-OD1	-6.15	112.77	118.30
1	C	236	PHE	CB-CG-CD1	6.14	125.10	120.80
1	A	251	TYR	CB-CG-CD1	6.09	124.66	121.00
1	A	172	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	D	121	TYR	CB-CG-CD2	6.08	124.64	121.00
1	A	291	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	C	189	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	A	17	GLU	OE1-CD-OE2	-5.96	116.14	123.30
1	A	268	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	268	ARG	NH1-CZ-NH2	-5.93	112.88	119.40
1	D	325	GLN	N-CA-CB	-5.92	99.94	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASP	OD1-CG-OD2	-5.91	112.07	123.30
1	C	172	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	260	PRO	N-CA-CB	5.87	110.35	103.30
1	A	322	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	338	ARG	CG-CD-NE	-5.87	99.47	111.80
1	D	268	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
1	A	28	GLN	N-CA-CB	5.83	121.09	110.60
1	B	172	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	209	PHE	CG-CD1-CE1	-5.79	114.43	120.80
1	D	291	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	D	96	SER	CB-CA-C	-5.78	99.11	110.10
1	A	144	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	B	279	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	192	TYR	CZ-CE2-CD2	-5.76	114.62	119.80
1	A	192	TYR	CB-CG-CD2	5.75	124.45	121.00
1	A	35	ASP	N-CA-CB	-5.73	100.28	110.60
1	B	342	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	C	268	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	182	SER	N-CA-CB	-5.72	101.92	110.50
1	A	89	PHE	CB-CG-CD1	-5.71	116.80	120.80
1	C	20	THR	CA-CB-OG1	-5.71	97.00	109.00
1	D	126	ASP	N-CA-CB	-5.68	100.38	110.60
1	C	34	ILE	C-N-CA	5.67	135.87	121.70
1	D	337	GLN	O-C-N	-5.67	113.63	122.70
1	A	57	GLN	O-C-N	5.64	131.73	122.70
1	B	177	VAL	O-C-N	-5.64	113.68	122.70
1	B	35	ASP	OD1-CG-OD2	5.60	133.94	123.30
1	D	260	PRO	C-N-CA	5.57	135.62	121.70
1	B	282	LEU	CB-CG-CD1	-5.53	101.61	111.00
1	A	50	LYS	N-CA-CB	5.52	120.54	110.60
1	A	305	GLU	CA-CB-CG	-5.51	101.28	113.40
1	C	78	GLN	CG-CD-OE1	-5.51	110.59	121.60
1	C	247	ASN	CA-CB-CG	5.51	125.52	113.40
1	C	265	TYR	CB-CG-CD2	-5.51	117.70	121.00
1	A	47	MET	CG-SD-CE	-5.49	91.41	100.20
1	C	217	GLU	CB-CA-C	-5.47	99.46	110.40
1	C	189	TYR	CZ-CE2-CD2	-5.46	114.88	119.80
1	B	202	ILE	CB-CA-C	5.45	122.51	111.60
1	A	304	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	C	125	PHE	CB-CG-CD1	-5.42	117.00	120.80
1	C	257	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	C	82	ASP	OD1-CG-OD2	-5.41	113.02	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	171	GLN	CG-CD-OE1	-5.40	110.79	121.60
1	A	23	SER	CA-CB-OG	-5.40	96.63	111.20
1	C	36	ALA	N-CA-CB	5.39	117.64	110.10
1	B	325	GLN	N-CA-CB	-5.38	100.92	110.60
1	C	322	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	175	VAL	CA-CB-CG2	-5.38	102.83	110.90
1	D	236	PHE	CD1-CG-CD2	-5.38	111.31	118.30
1	B	148	SER	N-CA-CB	-5.36	102.47	110.50
1	D	350	GLU	CG-CD-OE2	-5.35	107.60	118.30
1	C	307	ALA	CB-CA-C	5.34	118.11	110.10
1	B	58	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	219	VAL	CA-CB-CG2	-5.34	102.90	110.90
1	A	123	VAL	CG1-CB-CG2	5.33	119.42	110.90
1	A	334	GLU	C-N-CA	5.31	134.97	121.70
1	C	223	GLU	CB-CG-CD	-5.28	99.94	114.20
1	B	177	VAL	N-CA-CB	-5.26	99.93	111.50
1	D	216	GLY	CA-C-O	-5.26	111.14	120.60
1	D	221	THR	CA-CB-CG2	-5.25	105.05	112.40
1	A	241	TYR	CG-CD1-CE1	5.24	125.49	121.30
1	A	241	TYR	CD1-CE1-CZ	-5.23	115.09	119.80
1	B	223	GLU	O-C-N	5.22	131.06	122.70
1	A	28	GLN	O-C-N	5.21	131.04	122.70
1	B	203	GLY	N-CA-C	5.21	126.13	113.10
1	B	147	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	A	235	SER	N-CA-CB	-5.17	102.74	110.50
1	D	103	ALA	CB-CA-C	5.17	117.86	110.10
1	A	304	TYR	CA-CB-CG	-5.15	103.61	113.40
1	C	77	ASP	CB-CG-OD1	5.14	122.92	118.30
1	C	50	LYS	N-CA-CB	5.12	119.81	110.60
1	B	93	LEU	CA-CB-CG	-5.11	103.54	115.30
1	D	35	ASP	CB-CG-OD1	5.11	122.89	118.30
1	B	228	PRO	N-CA-CB	5.10	109.42	103.30
1	C	90	SER	N-CA-CB	5.10	118.15	110.50
1	A	96	SER	CB-CA-C	-5.10	100.42	110.10
1	A	27	GLN	CB-CG-CD	5.09	124.82	111.60
1	B	226	GLN	CA-CB-CG	-5.08	102.22	113.40
1	C	155	PRO	O-C-N	5.08	130.82	122.70
1	B	35	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	D	96	SER	O-C-N	-5.07	114.58	123.20
1	A	325	GLN	OE1-CD-NE2	5.07	133.55	121.90
1	A	138	VAL	CG1-CB-CG2	5.06	118.99	110.90
1	B	254	ASP	CB-CG-OD1	5.05	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	VAL	CG1-CB-CG2	-5.05	102.83	110.90
1	C	297	ASN	OD1-CG-ND2	5.03	133.47	121.90
1	B	117	TYR	O-C-N	-5.01	114.68	122.70
1	C	258	PRO	C-N-CA	-5.01	111.77	122.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	SER	Mainchain
1	A	170	GLU	Mainchain
1	A	217	GLU	Mainchain
1	A	224	ASN	Mainchain
1	A	26	LEU	Mainchain
1	B	314	GLU	Mainchain
1	B	316	ALA	Mainchain
1	B	91	ASN	Mainchain
1	C	318	GLY	Mainchain
1	D	185	LEU	Mainchain
1	D	35	ASP	Mainchain

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	2507	0	2420	57	0
1	B	2449	0	2374	31	3
1	C	2497	0	2428	54	0
1	D	2454	0	2376	48	0
2	A	40	0	0	0	3
2	B	56	0	0	2	0
2	C	47	0	0	2	0
2	D	52	0	0	2	0
All	All	10102	0	9598	174	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (174) 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:309:MET:HG2	2:B:409:HOH:O	1.51	1.10
1:A:105:GLU:HG2	1:A:106:GLU:HG3	1.31	1.06
1:A:154:LEU:H	1:A:155:PRO:CD	1.71	1.04
1:C:115:GLU:HB2	1:C:154:LEU:HD13	1.55	0.89
1:C:154:LEU:HD12	1:C:154:LEU:H	1.37	0.88
1:D:154:LEU:HD13	1:D:155:PRO:HD2	1.55	0.88
1:D:331:GLN:NE2	1:D:332:PRO:HD2	1.88	0.87
1:D:331:GLN:HE21	1:D:332:PRO:HD2	1.41	0.85
1:A:154:LEU:H	1:A:155:PRO:HD3	1.43	0.83
1:C:148:SER:HB2	1:C:185:LEU:HD11	1.58	0.82
1:A:152:GLU:CB	1:A:155:PRO:HG2	2.14	0.78
1:C:115:GLU:HB2	1:C:154:LEU:CD1	2.15	0.77
1:C:101:ILE:HD12	1:C:164:ASN:HB3	1.67	0.77
1:B:238:GLU:OE1	1:B:256:LYS:NZ	2.18	0.76
1:C:115:GLU:CB	1:C:154:LEU:HD13	2.18	0.74
1:B:19:ILE:HG23	1:B:220:LEU:HB3	1.70	0.73
1:A:214:LEU:HD22	1:C:214:LEU:HD22	1.71	0.72
1:B:33:ILE:HD12	1:B:204:LYS:HD2	1.71	0.70
1:C:309:MET:HG2	2:C:402:HOH:O	1.92	0.70
1:A:154:LEU:H	1:A:155:PRO:HD2	1.58	0.68
1:A:154:LEU:N	1:A:155:PRO:HD3	2.08	0.68
1:A:179:GLN:HG2	1:A:331:GLN:HE22	1.59	0.67
1:D:302:LEU:HD12	1:D:332:PRO:HG3	1.77	0.67
1:C:94:ARG:HG3	1:C:94:ARG:HH11	1.59	0.66
1:B:172:ARG:HH21	1:B:176:ASN:HD21	1.43	0.66
1:A:102:ILE:HD13	1:A:335:ILE:HD11	1.78	0.65
1:A:16:TYR:HE1	1:A:18:ILE:HG23	1.61	0.65
1:D:47:MET:HE2	1:D:51:GLN:HG3	1.79	0.65
1:D:236:PHE:CD2	1:D:252:ILE:HD11	2.32	0.64
1:C:163:ASP:O	1:C:165:THR:N	2.30	0.64
1:A:18:ILE:HD11	1:D:92:CYS:SG	2.38	0.64
1:D:154:LEU:CD1	1:D:155:PRO:HD2	2.28	0.63
1:A:105:GLU:HB3	1:A:108:ASP:OD2	1.99	0.63
1:A:115:GLU:OE1	1:A:155:PRO:HG3	1.98	0.62
1:C:61:ILE:HG23	1:C:65:THR:CB	2.30	0.62
1:C:305:GLU:O	1:C:309:MET:HG3	1.99	0.62
1:A:238:GLU:O	1:B:256:LYS:HE2	2.00	0.61
1:B:291:ARG:HD3	2:B:388:HOH:O	1.99	0.61
1:D:307:ALA:HB3	1:D:308:PRO:HD3	1.82	0.61
1:B:169:GLU:HG2	1:B:170:GLU:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:GLN:HE21	1:D:335:ILE:HG21	1.65	0.61
1:C:64:LEU:O	1:C:65:THR:C	2.39	0.61
1:C:225:LEU:HD23	1:C:226:GLN:N	2.16	0.60
1:C:61:ILE:HA	1:C:65:THR:HA	1.84	0.60
1:B:122:ILE:HG23	1:B:147:TYR:HB2	1.84	0.60
1:A:149:PRO:HB3	1:A:177:VAL:HG13	1.84	0.59
1:D:89:PHE:CZ	1:D:93:LEU:HD22	2.37	0.59
1:D:225:LEU:HD23	1:D:226:GLN:N	2.17	0.58
1:A:16:TYR:CE1	1:A:18:ILE:HG23	2.37	0.58
1:B:63:ASN:ND2	1:B:76:GLU:HA	2.19	0.58
1:D:251:TYR:CE1	1:D:255:LEU:HD11	2.37	0.58
1:A:238:GLU:OE1	1:A:256:LYS:NZ	2.34	0.57
1:B:289:TYR:OH	1:B:299:LYS:HD3	2.05	0.57
1:B:79:LYS:O	1:B:82:ASP:HB2	2.04	0.57
1:C:98:ARG:NH1	1:C:115:GLU:OE1	2.38	0.57
1:A:331:GLN:HE21	1:A:332:PRO:HD2	1.69	0.57
1:A:335:ILE:HG23	1:A:336:HIS:H	1.69	0.57
1:B:307:ALA:HB3	1:B:308:PRO:HD3	1.87	0.56
1:A:58:ARG:HG2	1:B:213:PRO:HD2	1.86	0.56
1:C:16:TYR:CB	1:C:19:ILE:HD11	2.35	0.56
1:D:288:GLY:HA3	2:D:401:HOH:O	2.06	0.56
1:A:79:LYS:O	1:A:82:ASP:HB2	2.06	0.56
1:A:209:PHE:HB3	1:A:218:PHE:HB3	1.89	0.55
1:A:331:GLN:NE2	1:A:332:PRO:HD2	2.22	0.55
1:D:225:LEU:HD11	1:D:282:LEU:HD23	1.89	0.55
1:C:225:LEU:HD11	1:C:282:LEU:HD23	1.88	0.54
1:D:169:GLU:OE1	1:D:172:ARG:NH2	2.40	0.54
1:C:102:ILE:HG23	1:C:171:GLN:NE2	2.23	0.54
1:D:236:PHE:CE2	1:D:252:ILE:HD11	2.43	0.54
1:B:94:ARG:HG2	1:C:16:TYR:N	2.23	0.53
1:C:290:PRO:HB3	1:C:342:TYR:OH	2.09	0.53
1:C:43:SER:O	1:C:47:MET:HG3	2.09	0.52
1:D:267:ALA:O	1:D:268:ARG:HD3	2.10	0.52
1:D:47:MET:CE	1:D:51:GLN:HG3	2.39	0.52
1:C:23:SER:O	1:C:27:GLN:HG3	2.10	0.51
1:C:154:LEU:HD12	1:C:154:LEU:N	2.16	0.51
1:A:257:GLU:OE2	1:B:242:LYS:HE3	2.11	0.51
1:C:331:GLN:NE2	1:C:332:PRO:HD2	2.26	0.51
1:A:222:GLN:HG3	1:A:223:GLU:N	2.26	0.50
1:A:307:ALA:HB3	1:A:308:PRO:HD3	1.93	0.50
1:D:336:HIS:HE1	2:D:408:HOH:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:HG2	1:A:128:LEU:H	1.77	0.50
1:B:169:GLU:HG2	1:B:170:GLU:H	1.76	0.49
1:A:149:PRO:HB3	1:A:177:VAL:CG1	2.43	0.49
1:D:244:TRP:CZ3	1:D:252:ILE:HG13	2.48	0.48
1:C:175:VAL:HG21	1:C:335:ILE:HA	1.94	0.48
1:C:238:GLU:OE1	1:C:256:LYS:NZ	2.26	0.48
1:B:24:TRP:O	1:B:28:GLN:HG2	2.14	0.48
1:A:215:TYR:CZ	1:D:51:GLN:HG2	2.49	0.48
1:D:302:LEU:CD1	1:D:332:PRO:HG3	2.44	0.48
1:D:28:GLN:OE1	1:D:33:ILE:HD12	2.13	0.48
1:A:115:GLU:OE1	1:A:155:PRO:CG	2.62	0.48
1:A:168:THR:HG21	1:A:172:ARG:NH2	2.29	0.48
1:B:172:ARG:HH21	1:B:176:ASN:ND2	2.11	0.47
1:C:84:ILE:O	1:C:88:VAL:HG23	2.13	0.47
1:D:148:SER:HB2	1:D:185:LEU:HD11	1.94	0.47
1:A:147:TYR:CZ	1:A:184:LEU:HD13	2.49	0.47
1:D:35:ASP:HB3	1:D:38:LEU:H	1.79	0.47
1:A:168:THR:HG22	1:A:172:ARG:CZ	2.44	0.47
1:C:123:VAL:HG22	1:C:146:ILE:HG12	1.97	0.47
1:C:162:ASP:HA	1:C:164:ASN:HB2	1.97	0.47
1:B:167:GLY:N	1:B:170:GLU:OE2	2.48	0.46
1:A:115:GLU:OE1	1:A:155:PRO:HD3	2.14	0.46
1:C:101:ILE:CD1	1:C:164:ASN:HB3	2.40	0.46
1:D:331:GLN:NE2	1:D:332:PRO:CD	2.72	0.46
1:C:29:GLU:HA	1:C:34:ILE:O	2.16	0.46
1:A:17:GLU:OE2	1:A:19:ILE:HD11	2.17	0.45
1:C:65:THR:CB	1:D:18:ILE:HG13	2.46	0.45
1:C:241:TYR:HA	1:C:244:TRP:CE3	2.52	0.45
1:A:215:TYR:CG	1:D:47:MET:HE1	2.52	0.45
1:C:291:ARG:HD2	1:C:296:LYS:O	2.17	0.45
1:A:349:VAL:O	1:A:353:GLU:HG3	2.17	0.45
1:C:115:GLU:OE1	1:C:154:LEU:HD12	2.16	0.45
1:A:148:SER:HB2	1:A:185:LEU:HD11	1.98	0.45
1:B:248:LEU:O	1:B:251:TYR:HB3	2.17	0.45
1:C:309:MET:CG	2:C:402:HOH:O	2.60	0.45
1:A:152:GLU:CB	1:A:155:PRO:CG	2.93	0.44
1:D:302:LEU:HA	1:D:306:CYS:HB2	1.98	0.44
1:A:215:TYR:CD1	1:D:47:MET:HE1	2.53	0.44
1:A:217:GLU:OE2	1:D:50:LYS:NZ	2.50	0.44
1:A:244:TRP:CG	1:A:248:LEU:HD23	2.52	0.44
1:D:24:TRP:O	1:D:28:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:MET:HE1	1:D:51:GLN:HE21	1.83	0.44
1:A:16:TYR:HE1	1:A:18:ILE:CG2	2.30	0.44
1:C:115:GLU:OE1	1:C:154:LEU:CD1	2.66	0.44
1:A:61:ILE:O	1:A:64:LEU:HB2	2.17	0.44
1:B:310:SER:O	1:B:313:VAL:HG12	2.18	0.44
1:A:225:LEU:HD11	1:A:282:LEU:HD23	1.99	0.43
1:C:305:GLU:O	1:C:308:PRO:HD2	2.18	0.43
1:D:331:GLN:HA	1:D:332:PRO:HD3	1.75	0.43
1:B:301:ARG:HD2	1:B:304:TYR:HD2	1.83	0.43
1:C:63:ASN:ND2	1:C:76:GLU:HA	2.34	0.43
1:D:244:TRP:HZ3	1:D:252:ILE:HG13	1.82	0.43
1:C:208:VAL:HB	1:C:222:GLN:HB3	2.00	0.43
1:A:51:GLN:O	1:A:55:LEU:HG	2.19	0.43
1:B:47:MET:CE	1:C:18:ILE:HD11	2.49	0.43
1:B:51:GLN:OE1	1:B:88:VAL:HG13	2.19	0.43
1:C:133:ASN:HB3	1:D:283:TYR:OH	2.19	0.43
1:D:326:ARG:HH11	1:D:326:ARG:HD3	1.50	0.43
1:A:104:SER:HB2	1:A:108:ASP:O	2.19	0.43
1:D:352:VAL:O	1:D:356:LEU:HG	2.19	0.43
1:B:96:SER:O	1:B:116:SER:HA	2.19	0.43
1:C:154:LEU:CD1	1:C:154:LEU:H	2.07	0.43
1:A:304:TYR:OH	1:A:335:ILE:HD12	2.18	0.42
1:A:89:PHE:CE1	1:A:93:LEU:HD13	2.53	0.42
1:C:166:LEU:HD13	1:C:174:ILE:HD12	2.01	0.42
1:D:47:MET:CE	1:D:51:GLN:HE21	2.32	0.42
1:D:91:ASN:HA	1:D:94:ARG:NH1	2.34	0.42
1:A:225:LEU:HD23	1:A:225:LEU:C	2.39	0.42
1:B:19:ILE:HG21	1:B:220:LEU:HD23	2.01	0.42
1:A:171:GLN:HB3	1:A:335:ILE:HD13	2.01	0.42
1:B:155:PRO:HD3	1:B:170:GLU:HG2	2.01	0.42
1:C:220:LEU:HD21	1:C:223:GLU:CG	2.49	0.42
1:C:120:ASN:O	1:C:149:PRO:HD2	2.19	0.42
1:D:301:ARG:HH11	1:D:336:HIS:HD2	1.68	0.42
1:C:256:LYS:HD3	1:D:241:TYR:HB3	2.02	0.42
1:D:122:ILE:HD13	1:D:122:ILE:HG21	1.89	0.41
1:D:53:ALA:O	1:D:57:GLN:HG3	2.20	0.41
1:A:242:LYS:HE3	1:B:257:GLU:OE2	2.20	0.41
1:D:331:GLN:HE21	1:D:332:PRO:CD	2.23	0.41
1:A:313:VAL:HG11	1:A:343:ILE:HG13	2.02	0.41
1:C:213:PRO:HD2	1:D:58:ARG:HG2	2.02	0.41
1:C:94:ARG:CG	1:C:94:ARG:HH11	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:SER:O	1:A:183:ASN:ND2	2.52	0.41
1:A:255:LEU:HD22	1:A:265:TYR:CE2	2.56	0.41
1:C:273:LEU:HD21	1:C:309:MET:SD	2.61	0.41
1:D:221:THR:O	1:D:222:GLN:HB2	2.20	0.41
1:A:122:ILE:HD12	1:A:149:PRO:HB3	2.03	0.40
1:B:154:LEU:HA	1:B:155:PRO:HD3	1.99	0.40
1:C:168:THR:HG22	1:C:169:GLU:OE1	2.21	0.40
1:C:247:ASN:HB3	1:C:355:TYR:O	2.22	0.40
1:A:97:GLY:HA3	1:A:114:GLU:OE2	2.22	0.40
1:B:166:LEU:HD23	1:B:166:LEU:HA	1.83	0.40
1:C:273:LEU:HD11	1:C:309:MET:CE	2.51	0.40

All (3) 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:B:202:ILE:O	2:A:382:HOH:O[2_656]	1.50	0.70
1:B:202:ILE:C	2:A:382:HOH:O[2_656]	2.07	0.13
1:B:203:GLY:N	2:A:382:HOH:O[2_656]	2.13	0.07

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	324/357 (91%)	305 (94%)	12 (4%)	7 (2%)	8 4
1	B	317/357 (89%)	306 (96%)	10 (3%)	1 (0%)	44 49
1	C	322/357 (90%)	306 (95%)	13 (4%)	3 (1%)	20 18
1	D	319/357 (89%)	304 (95%)	13 (4%)	2 (1%)	28 29
All	All	1282/1428 (90%)	1221 (95%)	48 (4%)	13 (1%)	18 16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	THR
1	A	154	LEU
1	A	335	ILE
1	C	155	PRO
1	C	163	ASP
1	C	164	ASN
1	D	18	ILE
1	D	106	GLU
1	A	105	GLU
1	A	14	SER
1	A	66	GLY
1	A	106	GLU
1	B	202	ILE

5.3.2 Protein sidechains ⓘ

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	272/307 (89%)	260 (96%)	12 (4%)	33	40
1	B	264/307 (86%)	255 (97%)	9 (3%)	42	53
1	C	270/307 (88%)	259 (96%)	11 (4%)	35	44
1	D	264/307 (86%)	251 (95%)	13 (5%)	29	35
All	All	1070/1228 (87%)	1025 (96%)	45 (4%)	34	43

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	19	ILE
1	A	47	MET
1	A	81	LEU
1	A	90	SER
1	A	116	SER
1	A	177	VAL
1	A	222	GLN
1	A	247	ASN

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Mol	Chain	Res	Type
1	A	289	TYR
1	A	299	LYS
1	A	313	VAL
1	B	33	ILE
1	B	47	MET
1	B	95	SER
1	B	116	SER
1	B	150	ASN
1	B	217	GLU
1	B	246	GLU
1	B	289	TYR
1	B	321	SER
1	C	18	ILE
1	C	64	LEU
1	C	93	LEU
1	C	98	ARG
1	C	126	ASP
1	C	150	ASN
1	C	154	LEU
1	C	204	LYS
1	C	230	SER
1	C	247	ASN
1	C	309	MET
1	D	18	ILE
1	D	35	ASP
1	D	126	ASP
1	D	154	LEU
1	D	155	PRO
1	D	182	SER
1	D	195	SER
1	D	201	THR
1	D	261	SER
1	D	266	SER
1	D	289	TYR
1	D	293	LYS
1	D	313	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	150	ASN

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Mol	Chain	Res	Type
1	A	164	ASN
1	A	176	ASN
1	A	240	ASN
1	A	331	GLN
1	B	63	ASN
1	B	78	GLN
1	B	176	ASN
1	B	240	ASN
1	B	331	GLN
1	B	336	HIS
1	C	63	ASN
1	C	78	GLN
1	C	164	ASN
1	C	171	GLN
1	C	176	ASN
1	C	240	ASN
1	C	331	GLN
1	D	51	GLN
1	D	63	ASN
1	D	78	GLN
1	D	164	ASN
1	D	171	GLN
1	D	176	ASN
1	D	240	ASN
1	D	331	GLN
1	D	336	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/357 (92%)	0.51	32 (9%) 8 7	21, 40, 74, 93	0
1	B	323/357 (90%)	0.22	17 (5%) 27 26	21, 34, 70, 96	0
1	C	328/357 (91%)	0.32	24 (7%) 16 15	23, 39, 71, 90	0
1	D	325/357 (91%)	0.41	34 (10%) 7 6	23, 38, 68, 97	0
All	All	1306/1428 (91%)	0.37	107 (8%) 12 11	21, 38, 72, 97	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157	PHE	9.5
1	D	260	PRO	9.0
1	D	105	GLU	8.8
1	A	260	PRO	8.8
1	D	259	GLY	8.8
1	A	67	THR	8.7
1	B	260	PRO	8.1
1	A	155	PRO	8.0
1	C	65	THR	7.5
1	A	259	GLY	7.2
1	C	64	LEU	7.0
1	A	14	SER	7.0
1	D	65	THR	6.9
1	B	262	GLY	6.4
1	D	262	GLY	6.3
1	B	259	GLY	6.2
1	C	16	TYR	6.2
1	A	12	LYS	6.1
1	A	262	GLY	6.1
1	D	66	GLY	6.0
1	A	261	SER	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	76	GLU	5.9
1	A	66	GLY	5.9
1	A	65	THR	5.5
1	C	156	ASP	4.7
1	C	162	ASP	4.5
1	D	261	SER	4.5
1	D	163	ASP	4.4
1	C	260	PRO	4.4
1	A	76	GLU	4.3
1	A	15	GLY	4.3
1	D	17	GLU	4.3
1	B	104	SER	4.2
1	B	261	SER	4.2
1	D	247	ASN	4.2
1	A	16	TYR	4.2
1	D	357	ALA	4.2
1	D	64	LEU	4.1
1	B	76	GLU	4.0
1	D	150	ASN	4.0
1	A	13	ARG	3.9
1	A	107	GLU	3.9
1	B	150	ASN	3.9
1	A	150	ASN	3.8
1	D	155	PRO	3.8
1	D	76	GLU	3.8
1	C	357	ALA	3.7
1	A	247	ASN	3.5
1	A	164	ASN	3.5
1	D	154	LEU	3.5
1	B	105	GLU	3.5
1	D	106	GLU	3.4
1	D	258	PRO	3.4
1	C	163	ASP	3.4
1	D	104	SER	3.2
1	A	105	GLU	3.2
1	A	106	GLU	3.1
1	D	151	ASP	3.0
1	C	155	PRO	3.0
1	C	150	ASN	3.0
1	B	163	ASP	3.0
1	D	296	LYS	2.9
1	C	259	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	169	GLU	2.8
1	A	331	GLN	2.8
1	C	105	GLU	2.8
1	D	35	ASP	2.7
1	D	252	ILE	2.6
1	D	246	GLU	2.6
1	C	169	GLU	2.6
1	C	94	ARG	2.5
1	C	236	PHE	2.5
1	D	89	PHE	2.5
1	A	131	SER	2.5
1	A	108	ASP	2.5
1	A	151	ASP	2.5
1	D	149	PRO	2.4
1	C	106	GLU	2.4
1	D	45	ILE	2.4
1	C	107	GLU	2.4
1	D	27	GLN	2.4
1	B	17	GLU	2.3
1	D	18	ILE	2.3
1	D	143	ILE	2.3
1	D	117	TYR	2.2
1	C	124	VAL	2.2
1	C	247	ASN	2.2
1	B	263	LYS	2.2
1	C	154	LEU	2.2
1	C	45	ILE	2.2
1	A	182	SER	2.2
1	B	64	LEU	2.2
1	A	124	VAL	2.2
1	B	294	LYS	2.2
1	B	291	ARG	2.2
1	D	93	LEU	2.1
1	A	79	LYS	2.1
1	A	179	GLN	2.1
1	C	252	ILE	2.1
1	D	42	LEU	2.1
1	B	357	ALA	2.1
1	A	35	ASP	2.0
1	A	143	ILE	2.0
1	B	258	PRO	2.0
1	A	77	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	123	VAL	2.0
1	D	63	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.