



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:47 PM UTC

PDB ID : 2ZF5 / pdb_00002zf5
Title : Crystal Structure of highly thermostable glycerol kinase from a hyperthermophilic archaeon
Authors : Koga, Y.; Katsumi, R.; You, D.-J.; Matsumura, H.; Takano, K.; Kanaya, S.
Deposited on : 2007-12-20
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

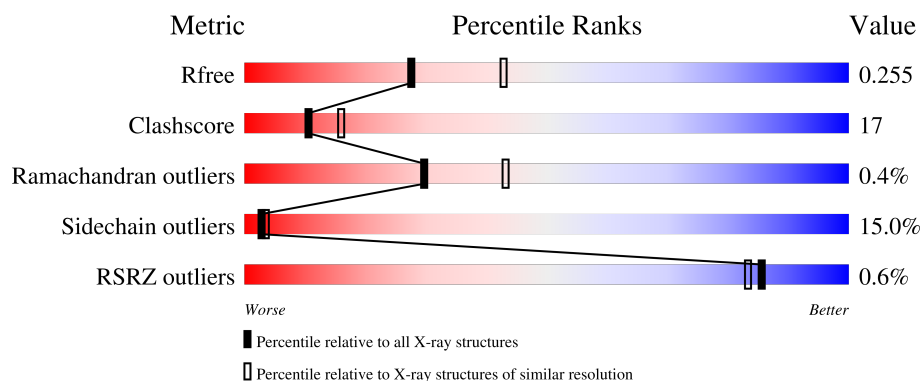
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	O	497	% 56% 33% 9% ..
1	Y	497	% 53% 34% 10% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7975 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	494	Total	C	N	O	S	0	0	0
			3921	2505	663	741	12			
1	Y	494	Total	C	N	O	S	0	0	0
			3921	2505	663	741	12			

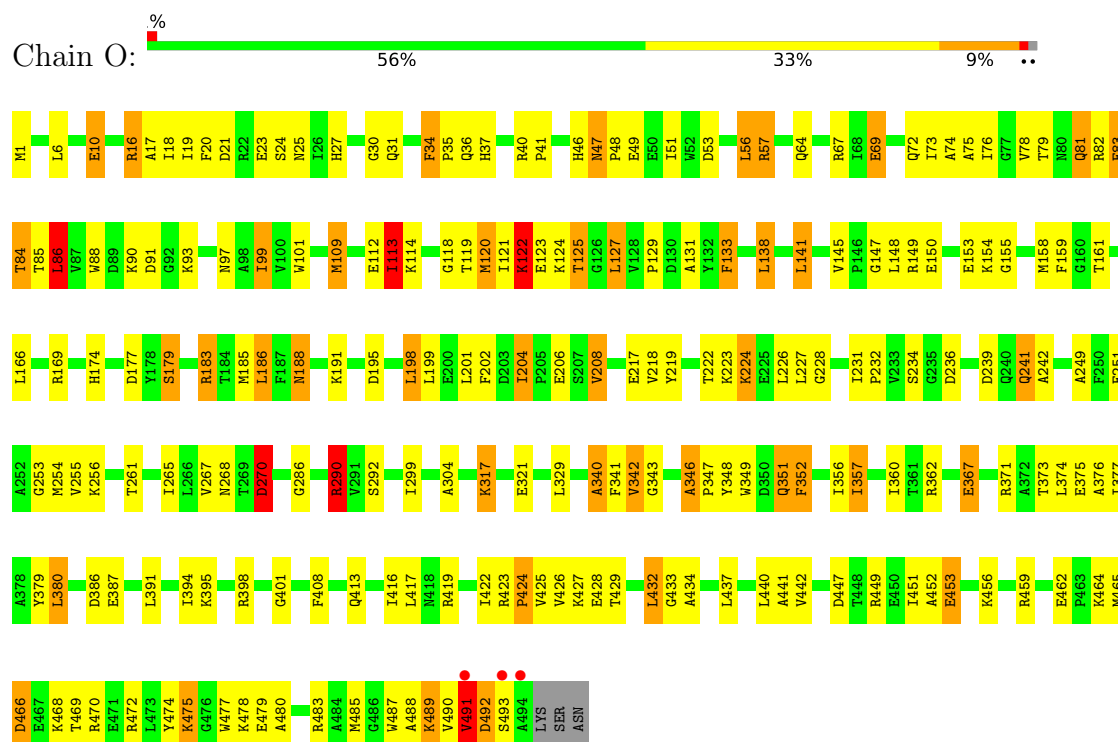
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	O	68	Total	O	0	0
			68	68		
2	Y	65	Total	O	0	0
			65	65		

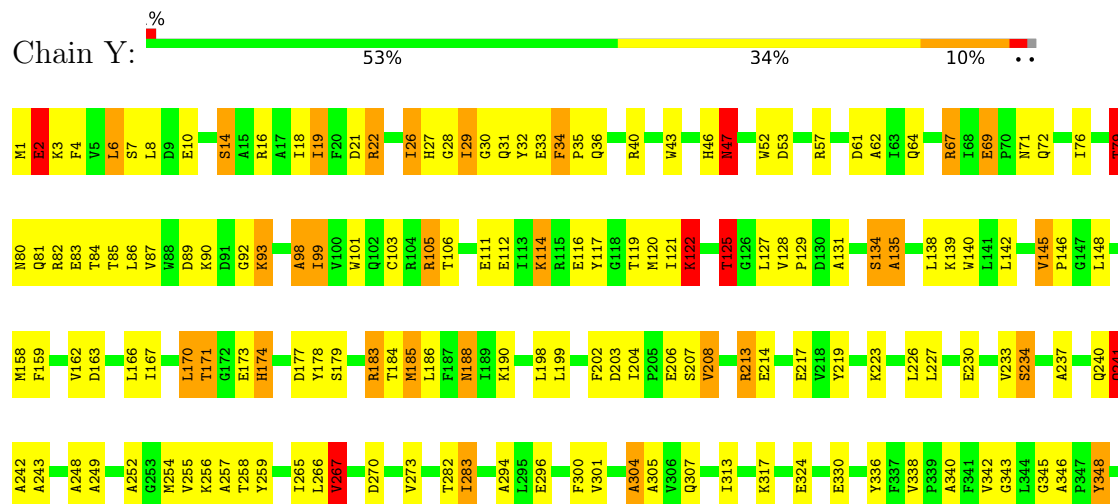
3 Residue-property plots

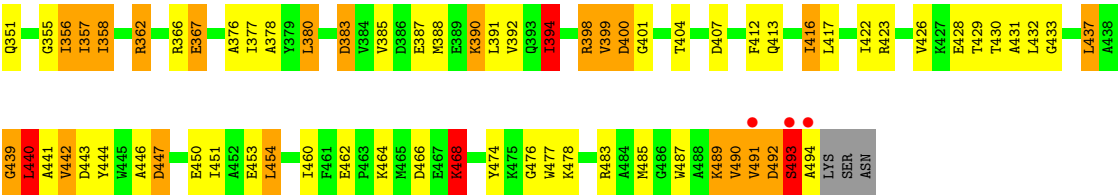
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycerol kinase



• Molecule 1: Glycerol kinase





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	217.48Å 217.48Å 66.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.10 – 2.40 41.10 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (41.10-2.40) 98.2 (41.10-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.174 , 0.255 0.173 , 0.255	Depositor DCC
R_{free} test set	2274 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7975	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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	O	1.74	31/4003 (0.8%)	1.65	62/5422 (1.1%)
1	Y	1.67	42/4003 (1.0%)	1.59	56/5422 (1.0%)
All	All	1.71	73/8006 (0.9%)	1.62	118/10844 (1.1%)

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	O	1	2
1	Y	1	2
All	All	2	4

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	270	ASP	CA-C	-10.47	1.43	1.53
1	Y	494	ALA	N-CA	9.05	1.63	1.46
1	Y	385	VAL	CA-CB	-8.18	1.44	1.54
1	O	451	ILE	CA-CB	-7.50	1.45	1.54
1	Y	252	ALA	CA-CB	-7.37	1.41	1.53
1	Y	493	SER	N-CA	7.35	1.55	1.46
1	Y	128	VAL	CA-CB	7.15	1.63	1.54
1	O	154	LYS	CA-C	6.91	1.62	1.52
1	Y	122	LYS	C-O	-6.70	1.16	1.24
1	O	83	GLU	N-CA	6.58	1.55	1.45
1	Y	273	VAL	CA-CB	6.55	1.62	1.53
1	O	51	ILE	CA-CB	6.55	1.61	1.54
1	O	84	THR	N-CA	-6.43	1.38	1.46
1	Y	243	ALA	C-O	-6.42	1.16	1.24
1	Y	84	THR	N-CA	-6.41	1.38	1.46
1	O	101	TRP	CA-C	6.33	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	441	ALA	N-CA	-6.27	1.37	1.46
1	Y	494	ALA	CA-CB	6.26	1.73	1.52
1	Y	342	VAL	CA-CB	6.24	1.62	1.54
1	O	480	ALA	CA-CB	-6.14	1.43	1.53
1	O	20	PHE	CA-C	6.13	1.60	1.52
1	Y	257	ALA	N-CA	-6.13	1.38	1.46
1	O	37	HIS	CA-CB	6.12	1.61	1.53
1	Y	257	ALA	CA-C	-6.08	1.45	1.52
1	Y	358	ILE	CA-C	6.07	1.59	1.52
1	Y	294	ALA	CA-CB	-6.01	1.43	1.53
1	O	86	LEU	C-O	-5.97	1.16	1.23
1	O	239	ASP	C-O	-5.91	1.17	1.24
1	Y	174	HIS	CA-C	5.90	1.60	1.53
1	O	360	ILE	CA-C	5.89	1.59	1.52
1	O	183	ARG	CD-NE	-5.87	1.38	1.46
1	Y	145	VAL	CA-CB	5.83	1.61	1.54
1	O	99	ILE	C-O	-5.80	1.17	1.23
1	Y	493	SER	CA-C	5.79	1.60	1.52
1	Y	390	LYS	C-O	5.78	1.31	1.24
1	Y	400	ASP	N-CA	5.70	1.53	1.45
1	O	267	VAL	CA-CB	5.69	1.61	1.54
1	O	379	TYR	N-CA	5.67	1.53	1.46
1	Y	283	ILE	CA-C	-5.63	1.45	1.52
1	O	267	VAL	C-O	5.56	1.30	1.24
1	Y	240	GLN	N-CA	-5.53	1.39	1.46
1	O	20	PHE	N-CA	5.52	1.52	1.45
1	O	340	ALA	CA-CB	5.49	1.59	1.52
1	O	362	ARG	CZ-NH2	5.48	1.40	1.33
1	O	161	THR	CA-CB	5.46	1.61	1.53
1	Y	437	LEU	C-O	-5.45	1.17	1.24
1	Y	394	ILE	CG1-CD1	-5.45	1.30	1.51
1	Y	304	ALA	CA-CB	5.40	1.62	1.53
1	Y	248	ALA	CA-CB	5.39	1.61	1.53
1	Y	426	VAL	CA-CB	5.39	1.59	1.53
1	Y	101	TRP	N-CA	5.38	1.52	1.46
1	Y	203	ASP	CB-CG	5.35	1.65	1.52
1	Y	345	GLY	C-O	-5.34	1.17	1.24
1	O	453	GLU	CA-C	5.34	1.60	1.52
1	Y	366	ARG	CA-C	5.32	1.59	1.52
1	Y	135	ALA	CA-CB	-5.32	1.45	1.53
1	Y	336	TYR	CA-C	5.31	1.59	1.52
1	O	113	ILE	CA-C	5.29	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	88	TRP	C-O	5.24	1.30	1.23
1	Y	447	ASP	C-O	5.21	1.30	1.23
1	Y	233	VAL	C-O	5.18	1.29	1.23
1	Y	34	PHE	N-CA	-5.18	1.41	1.45
1	Y	383	ASP	C-O	-5.17	1.18	1.24
1	Y	98	ALA	CA-CB	-5.15	1.45	1.53
1	O	265	ILE	C-O	-5.13	1.18	1.24
1	Y	346	ALA	N-CA	5.12	1.52	1.45
1	Y	392	VAL	N-CA	-5.10	1.39	1.46
1	O	41	PRO	N-CA	5.09	1.53	1.47
1	O	346	ALA	C-O	-5.09	1.17	1.24
1	Y	357	ILE	CB-CG2	5.09	1.69	1.52
1	O	299	ILE	CA-CB	5.07	1.60	1.54
1	O	425	VAL	CA-CB	5.07	1.60	1.54
1	Y	2	GLU	CA-C	5.03	1.59	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	82	ARG	CA-C-N	-18.00	93.98	122.23
1	O	82	ARG	C-N-CA	-18.00	93.98	122.23
1	Y	82	ARG	CA-C-N	-12.31	103.14	121.98
1	Y	82	ARG	C-N-CA	-12.31	103.14	121.98
1	O	492	ASP	N-CA-C	11.38	126.31	109.59
1	Y	34	PHE	CA-C-N	11.30	131.06	119.76
1	Y	34	PHE	C-N-CA	11.30	131.06	119.76
1	O	441	ALA	N-CA-C	9.98	124.99	113.01
1	O	270	ASP	N-CA-C	9.45	122.68	108.31
1	O	491	VAL	CA-C-N	9.19	134.48	121.24
1	O	491	VAL	C-N-CA	9.19	134.48	121.24
1	Y	71	ASN	N-CA-C	-8.98	102.31	113.18
1	Y	270	ASP	CB-CA-C	8.81	127.95	110.42
1	Y	125	THR	N-CA-CB	-8.74	97.87	110.81
1	O	82	ARG	O-C-N	-8.70	110.53	122.46
1	O	219	TYR	N-CA-C	-8.61	102.91	113.50
1	Y	401	GLY	N-CA-C	-8.55	103.44	112.08
1	Y	267	VAL	CB-CA-C	-8.48	97.92	110.81
1	O	183	ARG	CB-CG-CD	-8.03	92.83	111.30
1	Y	493	SER	N-CA-C	-8.01	93.74	110.80
1	Y	493	SER	CA-C-N	-7.03	109.04	121.70
1	Y	493	SER	C-N-CA	-7.03	109.04	121.70
1	O	267	VAL	CB-CA-C	-6.98	101.35	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	206	GLU	N-CA-C	6.96	120.66	111.75
1	Y	82	ARG	N-CA-C	6.91	121.87	113.17
1	O	30	GLY	N-CA-C	-6.83	100.25	111.38
1	O	40	ARG	CA-C-N	-6.81	112.75	119.90
1	O	40	ARG	C-N-CA	-6.81	112.75	119.90
1	Y	340	ALA	N-CA-C	-6.76	101.28	110.68
1	O	82	ARG	N-CA-C	6.74	121.59	113.23
1	Y	69	GLU	CA-C-N	-6.70	113.25	119.82
1	Y	69	GLU	C-N-CA	-6.70	113.25	119.82
1	Y	2	GLU	CB-CA-C	6.68	120.82	109.53
1	Y	183	ARG	CB-CG-CD	-6.67	95.95	111.30
1	Y	447	ASP	CB-CA-C	-6.64	98.01	110.16
1	O	34	PHE	CA-C-N	6.60	126.52	119.85
1	O	34	PHE	C-N-CA	6.60	126.52	119.85
1	O	155	GLY	N-CA-C	-6.50	105.70	115.32
1	Y	82	ARG	O-C-N	-6.49	114.23	122.34
1	Y	439	GLY	CA-C-N	-6.41	111.05	120.28
1	Y	439	GLY	C-N-CA	-6.41	111.05	120.28
1	Y	492	ASP	N-CA-C	6.41	124.45	110.80
1	Y	29	ILE	CB-CA-C	-6.41	100.44	110.69
1	Y	122	LYS	N-CA-C	-6.41	104.30	111.28
1	O	351	GLN	CB-CG-CD	6.35	123.39	112.60
1	Y	348	TYR	N-CA-C	6.11	117.74	111.14
1	O	475	LYS	N-CA-C	-6.09	104.55	112.23
1	Y	468	LYS	CA-C-N	6.08	128.70	120.44
1	Y	468	LYS	C-N-CA	6.08	128.70	120.44
1	Y	440	LEU	CA-CB-CG	6.07	137.56	116.30
1	Y	343	GLY	N-CA-C	-6.05	103.69	112.17
1	Y	305	ALA	N-CA-C	-6.03	104.83	111.82
1	O	479	GLU	N-CA-C	-6.02	104.65	112.23
1	O	362	ARG	NE-CZ-NH1	-5.97	115.53	121.50
1	O	253	GLY	N-CA-C	-5.97	106.28	114.64
1	Y	489	LYS	N-CA-C	-5.92	103.44	111.55
1	Y	183	ARG	N-CA-C	5.88	120.06	113.01
1	O	387	GLU	N-CA-C	5.83	117.72	111.36
1	O	83	GLU	CA-C-N	5.80	132.00	121.97
1	O	83	GLU	C-N-CA	5.80	132.00	121.97
1	Y	446	ALA	N-CA-C	5.79	117.67	111.36
1	O	78	VAL	N-CA-C	5.77	116.25	108.17
1	O	206	GLU	N-CA-C	5.75	119.55	112.54
1	O	413	GLN	N-CA-C	5.74	118.00	111.11
1	O	352	PHE	N-CA-C	5.74	120.28	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	204	ILE	N-CA-C	5.72	114.17	107.77
1	O	56	LEU	N-CA-C	5.67	117.92	111.11
1	O	343	GLY	N-CA-C	-5.67	105.47	112.33
1	Y	134	SER	N-CA-C	5.65	117.89	111.11
1	Y	300	PHE	N-CA-C	5.65	117.44	111.28
1	Y	377	ILE	N-CA-C	-5.62	105.04	110.72
1	O	452	ALA	N-CA-C	5.60	118.11	111.33
1	Y	407	ASP	N-CA-C	5.57	117.35	111.28
1	O	133	PHE	N-CA-C	5.55	118.04	110.55
1	O	122	LYS	N-CA-C	-5.54	105.39	111.82
1	O	485	MET	CA-CB-CG	-5.52	103.07	114.10
1	O	386	ASP	N-CA-C	5.50	118.03	111.71
1	Y	185	MET	CG-SD-CE	-5.48	88.84	100.90
1	O	299	ILE	N-CA-C	-5.45	99.80	107.75
1	O	466	ASP	N-CA-C	5.43	117.89	110.55
1	Y	439	GLY	O-C-N	-5.42	116.99	122.19
1	Y	462	GLU	CA-C-N	-5.40	114.22	119.78
1	Y	462	GLU	C-N-CA	-5.40	114.22	119.78
1	O	422	ILE	CB-CA-C	-5.37	103.14	110.77
1	Y	241	GLN	CB-CG-CD	5.36	121.72	112.60
1	Y	47	ASN	CA-C-O	-5.36	115.81	119.29
1	Y	398	ARG	N-CA-C	-5.36	100.96	109.96
1	Y	79	THR	CB-CA-C	-5.36	98.78	109.33
1	Y	30	GLY	N-CA-C	-5.35	102.66	111.38
1	Y	145	VAL	CA-C-N	5.34	126.18	119.98
1	Y	145	VAL	C-N-CA	5.34	126.18	119.98
1	O	218	VAL	N-CA-CB	5.33	116.74	110.82
1	O	179	SER	N-CA-C	5.31	117.49	111.02
1	Y	40	ARG	CA-C-N	-5.30	114.46	119.76
1	Y	40	ARG	C-N-CA	-5.30	114.46	119.76
1	O	488	ALA	CA-C-N	-5.30	113.80	122.54
1	O	488	ALA	C-N-CA	-5.30	113.80	122.54
1	O	342	VAL	N-CA-C	5.29	120.34	109.34
1	O	493	SER	N-CA-C	-5.27	106.16	112.59
1	Y	61	ASP	N-CA-C	5.25	117.00	111.28
1	O	166	LEU	N-CA-C	5.24	116.99	111.28
1	O	491	VAL	N-CA-C	-5.23	102.03	109.51
1	Y	307	GLN	N-CA-C	-5.22	105.59	111.28
1	Y	398	ARG	CD-NE-CZ	5.17	131.64	124.40
1	Y	19	ILE	N-CA-C	-5.13	100.99	108.17
1	O	290	ARG	N-CA-C	5.13	117.60	109.50
1	O	489	LYS	N-CA-C	5.09	119.59	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	401	GLY	CA-C-N	5.08	125.72	120.03
1	O	401	GLY	C-N-CA	5.08	125.72	120.03
1	O	362	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	O	27	HIS	N-CA-C	-5.04	108.16	114.56
1	O	69	GLU	CA-C-N	5.04	125.06	119.32
1	O	69	GLU	C-N-CA	5.04	125.06	119.32
1	O	357	ILE	N-CA-C	-5.04	100.39	107.75
1	O	286	GLY	O-C-N	-5.03	120.18	123.35
1	O	186	LEU	N-CA-C	-5.02	107.11	114.39
1	O	93	LYS	CA-C-N	5.02	124.95	119.78
1	O	93	LYS	C-N-CA	5.02	124.95	119.78

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	O	270	ASP	CA
1	Y	270	ASP	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	491	VAL	Peptide
1	O	492	ASP	Peptide
1	Y	492	ASP	Peptide
1	Y	493	SER	Peptide

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	O	3921	0	3897	126	0
1	Y	3921	0	3897	142	0
2	O	68	0	0	2	0
2	Y	65	0	0	1	0
All	All	7975	0	7794	262	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 17.

All (262) 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:O:109:MET:HE2	1:O:113:ILE:HD12	1.29	1.13
1:Y:183:ARG:HH21	1:Y:282:THR:HG21	1.10	1.09
1:Y:159:PHE:HB3	1:Y:208:VAL:HG13	1.32	1.06
1:Y:489:LYS:O	1:Y:489:LYS:HG3	1.55	1.05
1:Y:125:THR:HG22	1:Y:127:LEU:H	1.22	1.05
1:Y:26:ILE:HD12	1:Y:28:GLY:H	1.21	1.04
1:Y:1:MET:HE3	1:Y:3:LYS:HE3	1.44	0.96
1:Y:171:THR:HG22	1:Y:173:GLU:H	1.28	0.95
1:O:57:ARG:HG3	1:O:57:ARG:HH11	1.30	0.94
1:Y:255:VAL:HG22	1:Y:267:VAL:HG13	1.50	0.93
1:O:16:ARG:NH1	1:O:428:GLU:OE1	2.01	0.93
1:Y:121:ILE:O	1:Y:125:THR:HB	1.70	0.91
1:Y:142:LEU:HD23	1:Y:148:LEU:HD23	1.54	0.89
1:Y:183:ARG:NH2	1:Y:282:THR:HG21	1.85	0.89
1:O:109:MET:HE2	1:O:113:ILE:CD1	2.03	0.88
1:Y:26:ILE:HD12	1:Y:28:GLY:N	1.90	0.87
1:Y:159:PHE:CB	1:Y:208:VAL:HG13	2.05	0.86
1:Y:121:ILE:HG21	1:Y:185:MET:HE2	1.58	0.85
1:Y:159:PHE:HB3	1:Y:208:VAL:CG1	2.07	0.84
1:Y:183:ARG:HH21	1:Y:282:THR:CG2	1.91	0.84
1:Y:129:PRO:HA	1:Y:185:MET:HE1	1.60	0.83
1:O:125:THR:CG2	1:O:127:LEU:HB2	2.09	0.82
1:Y:362:ARG:NH2	2:Y:537:HOH:O	2.08	0.80
1:Y:16:ARG:HG2	1:Y:31:GLN:HB3	1.62	0.80
1:O:224:LYS:O	1:O:228:GLY:N	2.14	0.80
1:O:120:MET:O	1:O:124:LYS:HG3	1.82	0.79
1:O:188:ASN:ND2	1:O:191:LYS:H	1.81	0.79
1:Y:1:MET:CE	1:Y:3:LYS:HE3	2.12	0.78
1:Y:213:ARG:HD2	1:Y:217:GLU:OE2	1.82	0.78
1:Y:67:ARG:HG3	1:Y:67:ARG:HH11	1.52	0.74
1:Y:47:ASN:HD22	1:Y:47:ASN:C	1.94	0.74
1:O:270:ASP:HB2	1:O:292:SER:OG	1.90	0.72
1:Y:19:ILE:HD13	1:Y:62:ALA:HB1	1.72	0.72
1:O:121:ILE:O	1:O:125:THR:HB	1.89	0.71
1:O:125:THR:HG23	1:O:127:LEU:HD22	1.72	0.71
1:O:255:VAL:HG21	1:O:394:ILE:HG23	1.71	0.71
1:Y:125:THR:CG2	1:Y:127:LEU:HB2	2.21	0.71
1:O:133:PHE:CD2	1:O:185:MET:HE3	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:69:GLU:H	1:O:72:GLN:NE2	1.90	0.70
1:Y:301:VAL:HG13	1:Y:304:ALA:HB3	1.71	0.70
1:Y:22:ARG:HD3	1:Y:444:TYR:O	1.91	0.70
1:O:487:TRP:CZ2	1:O:491:VAL:HG21	2.27	0.70
1:Y:489:LYS:O	1:Y:489:LYS:CG	2.37	0.70
1:O:158:MET:HE2	1:O:174:HIS:HB2	1.74	0.69
1:Y:234:SER:HB2	1:Y:441:ALA:HB3	1.73	0.69
1:Y:69:GLU:H	1:Y:72:GLN:HE21	1.41	0.68
1:Y:121:ILE:CG2	1:Y:185:MET:HE2	2.24	0.67
1:Y:103:CYS:SG	1:Y:105:ARG:HD2	2.35	0.67
1:O:47:ASN:C	1:O:47:ASN:HD22	2.02	0.67
1:Y:16:ARG:NH1	1:Y:428:GLU:OE1	2.28	0.67
1:Y:26:ILE:HG13	1:Y:26:ILE:O	1.95	0.67
1:Y:188:ASN:HD22	1:Y:190:LYS:H	1.42	0.67
1:O:125:THR:HG23	1:O:127:LEU:HB2	1.76	0.66
1:O:447:ASP:OD2	1:O:449:ARG:HB3	1.94	0.66
1:Y:21:ASP:OD2	1:Y:27:HIS:NE2	2.24	0.66
1:Y:79:THR:HG22	1:Y:237:ALA:O	1.96	0.65
1:Y:6:LEU:HD23	1:Y:76:ILE:HG12	1.79	0.65
1:O:159:PHE:HB3	1:O:208:VAL:HG13	1.80	0.64
1:O:380:LEU:HD13	1:O:477:TRP:HZ2	1.64	0.63
1:O:16:ARG:HG3	1:O:31:GLN:HB3	1.81	0.63
1:O:53:ASP:OD2	1:O:57:ARG:NH1	2.32	0.63
1:O:69:GLU:H	1:O:72:GLN:HE21	1.45	0.63
1:O:57:ARG:HH11	1:O:57:ARG:CG	2.10	0.63
1:Y:125:THR:HG22	1:Y:127:LEU:N	2.04	0.63
1:O:290:ARG:HH11	1:O:290:ARG:HB2	1.64	0.61
1:O:47:ASN:ND2	1:O:49:GLU:H	1.99	0.61
1:Y:142:LEU:HD23	1:Y:148:LEU:CD2	2.26	0.61
1:O:147:GLY:HA2	1:O:150:GLU:OE1	2.00	0.60
1:O:394:ILE:O	1:O:419:ARG:HD3	2.01	0.60
1:O:118:GLY:HA2	1:O:129:PRO:HG2	1.83	0.60
1:O:36:GLN:OE1	1:O:46:HIS:HE1	1.84	0.60
1:O:356:ILE:HG22	1:Y:358:ILE:HG13	1.84	0.59
1:O:6:LEU:HD23	1:O:76:ILE:HG12	1.84	0.59
1:O:138:LEU:HD13	1:O:204:ILE:HG12	1.85	0.59
1:Y:259:TYR:HE1	1:Y:399:VAL:HG22	1.68	0.59
1:O:122:LYS:HG2	1:O:127:LEU:O	2.03	0.58
1:O:149:ARG:O	1:O:153:GLU:HG3	2.03	0.58
1:Y:491:VAL:O	1:Y:491:VAL:CG1	2.51	0.58
1:O:79:THR:HB	1:O:434:ALA:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:26:ILE:CD1	1:Y:28:GLY:N	2.65	0.57
1:Y:134:SER:HB2	1:Y:184:THR:HA	1.85	0.57
1:O:133:PHE:CD2	1:O:185:MET:CE	2.87	0.57
1:Y:114:LYS:HG2	1:Y:129:PRO:HB2	1.86	0.57
1:Y:47:ASN:C	1:Y:47:ASN:ND2	2.62	0.57
1:Y:214:GLU:O	1:Y:219:TYR:OH	2.17	0.57
1:O:186:LEU:HD21	1:O:204:ILE:HD13	1.86	0.57
1:O:109:MET:CE	1:O:113:ILE:CD1	2.81	0.57
1:Y:422:ILE:HG12	1:Y:460:ILE:HG12	1.86	0.57
1:Y:367:GLU:CD	1:Y:367:GLU:H	2.13	0.56
1:Y:487:TRP:O	1:Y:490:VAL:HG12	2.05	0.56
1:O:17:ALA:C	1:O:18:ILE:HD12	2.30	0.56
1:O:179:SER:HB2	1:O:241:GLN:HG3	1.88	0.56
1:O:356:ILE:HA	1:Y:357:ILE:O	2.05	0.56
1:Y:171:THR:CG2	1:Y:173:GLU:H	2.10	0.55
1:Y:67:ARG:HG3	1:Y:67:ARG:NH1	2.21	0.55
1:O:21:ASP:OD1	1:O:23:GLU:N	2.38	0.55
1:Y:442:VAL:O	1:Y:442:VAL:HG13	2.07	0.54
1:Y:86:LEU:HD12	1:Y:86:LEU:N	2.22	0.54
1:O:224:LYS:O	1:O:228:GLY:CA	2.55	0.54
1:O:85:THR:C	1:O:86:LEU:HD12	2.32	0.54
1:Y:179:SER:HB2	1:Y:241:GLN:HG3	1.89	0.54
1:Y:188:ASN:ND2	1:Y:190:LYS:H	2.06	0.54
1:O:125:THR:HG22	1:O:127:LEU:H	1.74	0.53
1:O:21:ASP:OD1	1:O:21:ASP:C	2.50	0.53
1:O:491:VAL:HG22	1:Y:476:GLY:HA2	1.90	0.53
1:Y:26:ILE:CD1	1:Y:28:GLY:H	2.08	0.53
1:O:83:GLU:OE2	1:O:183:ARG:HD2	2.09	0.53
1:Y:177:ASP:HA	1:Y:213:ARG:O	2.07	0.53
1:O:47:ASN:C	1:O:47:ASN:ND2	2.67	0.53
1:O:226:LEU:HB3	1:O:227:LEU:HD22	1.90	0.53
1:Y:491:VAL:O	1:Y:491:VAL:HG12	2.08	0.53
1:O:424:PRO:HG2	1:O:426:VAL:O	2.09	0.52
1:Y:256:LYS:O	1:Y:265:ILE:HA	2.10	0.52
1:Y:348:TYR:OH	1:Y:383:ASP:OD2	2.24	0.52
1:Y:388:MET:HB3	1:Y:394:ILE:HD11	1.91	0.52
1:Y:105:ARG:HG2	1:Y:106:THR:HG23	1.92	0.51
1:O:158:MET:HE2	1:O:174:HIS:CG	2.45	0.51
1:O:141:LEU:O	1:O:145:VAL:HG23	2.09	0.51
1:Y:171:THR:HG22	1:Y:173:GLU:N	2.11	0.51
1:Y:324:GLU:CD	1:Y:324:GLU:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:86:LEU:HD12	1:O:86:LEU:N	2.26	0.51
1:Y:256:LYS:HD2	1:Y:256:LYS:C	2.36	0.51
1:Y:6:LEU:HD13	1:Y:19:ILE:HD11	1.92	0.51
1:Y:442:VAL:O	1:Y:442:VAL:CG1	2.59	0.50
1:O:487:TRP:CH2	1:O:491:VAL:HG21	2.47	0.50
1:Y:19:ILE:HD13	1:Y:62:ALA:CB	2.39	0.50
1:Y:265:ILE:C	1:Y:266:LEU:HD12	2.36	0.50
1:Y:178:TYR:HB3	1:Y:283:ILE:HG21	1.93	0.50
1:Y:242:ALA:O	1:Y:433:GLY:HA3	2.12	0.50
1:O:380:LEU:HD13	1:O:477:TRP:CZ2	2.46	0.50
1:Y:131:ALA:H	1:Y:351:GLN:NE2	2.09	0.49
1:O:21:ASP:OD2	1:O:25:ASN:HB2	2.12	0.49
1:O:73:ILE:HG22	1:O:231:ILE:HG21	1.95	0.49
1:Y:125:THR:CG2	1:Y:127:LEU:CB	2.90	0.49
1:Y:439:GLY:O	1:Y:440:LEU:C	2.46	0.49
1:O:217:GLU:O	1:O:234:SER:HA	2.12	0.49
1:Y:83:GLU:OE2	1:Y:183:ARG:HD2	2.12	0.49
1:O:47:ASN:HD22	1:O:49:GLU:N	2.11	0.49
1:O:109:MET:CE	1:O:113:ILE:HD12	2.21	0.49
1:O:133:PHE:HD2	1:O:185:MET:CE	2.25	0.49
1:Y:378:ALA:HB1	1:Y:416:ILE:HD11	1.95	0.49
1:Y:32:TYR:CE2	1:Y:57:ARG:NH1	2.81	0.49
1:O:352:PHE:CD2	1:O:489:LYS:HD3	2.49	0.48
1:Y:85:THR:HG23	1:Y:159:PHE:HE1	1.77	0.48
1:Y:404:THR:O	1:Y:423:ARG:NH1	2.45	0.48
1:O:158:MET:CE	1:O:174:HIS:HB2	2.41	0.48
1:O:202:PHE:HB2	1:O:204:ILE:HD12	1.95	0.48
1:Y:186:LEU:HD11	1:Y:204:ILE:HD13	1.96	0.48
1:Y:378:ALA:HA	1:Y:413:GLN:NE2	2.29	0.48
1:Y:387:GLU:HA	1:Y:390:LYS:HD3	1.96	0.48
1:O:10:GLU:CD	1:O:10:GLU:C	2.81	0.47
1:Y:79:THR:HG21	1:Y:242:ALA:HB3	1.96	0.47
1:O:24:SER:HB2	1:O:432:LEU:HD21	1.96	0.47
1:Y:255:VAL:HG21	1:Y:394:ILE:HG23	1.96	0.47
1:Y:85:THR:HG23	1:Y:159:PHE:CE1	2.48	0.47
1:Y:116:GLU:HB2	1:Y:117:TYR:CD2	2.50	0.47
1:Y:125:THR:HG23	1:Y:127:LEU:CG	2.45	0.47
1:Y:217:GLU:O	1:Y:234:SER:HA	2.14	0.47
1:Y:122:LYS:HG2	1:Y:127:LEU:O	2.15	0.47
1:Y:412:PHE:O	1:Y:416:ILE:HG13	2.15	0.47
1:O:270:ASP:CB	1:O:292:SER:OG	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:2:GLU:HG3	1:Y:4:PHE:CZ	2.50	0.47
1:O:47:ASN:ND2	1:O:49:GLU:N	2.62	0.46
1:Y:466:ASP:OD1	1:Y:468:LYS:HE3	2.15	0.46
1:O:47:ASN:HD22	1:O:49:GLU:H	1.64	0.46
1:Y:99:ILE:HD13	1:Y:105:ARG:CZ	2.45	0.46
1:Y:162:VAL:O	1:Y:166:LEU:HG	2.15	0.46
1:O:357:ILE:O	1:Y:356:ILE:HA	2.15	0.46
1:O:158:MET:HE2	1:O:174:HIS:CB	2.43	0.46
1:O:251:GLU:O	1:O:254:MET:HB2	2.16	0.46
1:Y:46:HIS:HB2	1:Y:98:ALA:HB3	1.98	0.46
1:Y:416:ILE:HG13	1:Y:416:ILE:H	1.58	0.46
1:Y:81:GLN:O	1:Y:81:GLN:HG3	2.16	0.45
1:Y:1:MET:HE3	1:Y:3:LYS:CE	2.30	0.45
1:O:465:MET:O	1:O:470:ARG:NH1	2.46	0.45
1:O:131:ALA:H	1:O:351:GLN:NE2	2.15	0.45
1:O:159:PHE:CB	1:O:208:VAL:HG13	2.46	0.45
1:Y:134:SER:O	1:Y:135:ALA:C	2.59	0.45
1:O:183:ARG:HA	1:O:183:ARG:HD3	1.72	0.45
1:O:329:LEU:HD12	1:O:371:ARG:HD3	1.98	0.45
1:O:256:LYS:HD2	1:O:256:LYS:C	2.41	0.45
1:O:367:GLU:CD	1:O:367:GLU:H	2.24	0.45
1:Y:87:VAL:HA	1:Y:158:MET:O	2.16	0.45
1:O:186:LEU:CD2	1:O:204:ILE:HD13	2.45	0.45
1:O:426:VAL:HG23	2:O:515:HOH:O	2.17	0.45
1:Y:89:ASP:O	1:Y:92:GLY:N	2.43	0.45
1:O:249:ALA:HA	1:O:254:MET:HE2	1.97	0.44
1:Y:22:ARG:HE	1:Y:22:ARG:HB2	1.41	0.44
1:Y:451:ILE:HA	1:Y:454:LEU:HD22	1.99	0.44
1:O:474:TYR:CD2	1:O:478:LYS:HD2	2.52	0.44
1:O:223:LYS:H	1:O:223:LYS:HG2	1.54	0.44
1:O:348:TYR:O	1:O:349:TRP:C	2.58	0.44
1:Y:79:THR:CG2	1:Y:237:ALA:O	2.65	0.44
1:Y:388:MET:CB	1:Y:394:ILE:HD11	2.46	0.44
1:O:129:PRO:HA	1:O:185:MET:HE1	1.99	0.44
1:Y:183:ARG:NH2	1:Y:282:THR:CG2	2.65	0.44
1:Y:158:MET:HE2	1:Y:174:HIS:HB2	2.00	0.44
1:O:133:PHE:HD2	1:O:185:MET:HE3	1.80	0.44
1:Y:14:SER:HA	1:Y:33:GLU:HA	2.00	0.44
1:Y:139:LYS:HG3	1:Y:202:PHE:O	2.17	0.44
1:O:317:LYS:HB2	1:O:321:GLU:OE2	2.18	0.43
1:O:483:ARG:O	1:Y:483:ARG:NH1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:167:ILE:O	1:Y:171:THR:HB	2.18	0.43
1:Y:249:ALA:HB1	1:Y:254:MET:HB2	2.00	0.43
1:O:371:ARG:O	1:O:375:GLU:HG3	2.18	0.43
1:Y:80:ASN:ND2	1:Y:163:ASP:HB3	2.32	0.43
1:Y:36:GLN:OE1	1:Y:46:HIS:HE1	2.02	0.43
1:O:81:GLN:NE2	1:O:84:THR:OG1	2.51	0.43
1:O:86:LEU:N	1:O:86:LEU:CD1	2.82	0.43
1:O:466:ASP:OD1	1:O:466:ASP:N	2.49	0.43
1:Y:145:VAL:HA	1:Y:146:PRO:HD3	1.74	0.43
1:Y:93:LYS:HB3	1:Y:93:LYS:HE2	1.64	0.43
1:O:236:ASP:OD1	1:O:236:ASP:C	2.61	0.43
1:O:74:ALA:O	1:O:232:PRO:HG2	2.19	0.43
1:O:188:ASN:HD22	1:O:191:LYS:H	1.62	0.43
1:O:456:LYS:N	2:O:561:HOH:O	2.08	0.43
1:Y:266:LEU:HD12	1:Y:266:LEU:N	2.34	0.43
1:Y:159:PHE:CB	1:Y:208:VAL:CG1	2.84	0.43
1:O:195:ASP:HB3	1:O:198:LEU:HD22	2.00	0.42
1:O:231:ILE:HG23	1:O:232:PRO:HD2	2.00	0.42
1:O:99:ILE:HD11	1:O:141:LEU:HD13	2.02	0.42
1:O:373:THR:O	1:O:377:ILE:HG13	2.19	0.42
1:Y:430:THR:O	1:Y:431:ALA:C	2.61	0.42
1:Y:490:VAL:HG22	1:Y:490:VAL:O	2.19	0.42
1:Y:34:PHE:HA	1:Y:35:PRO:HD3	1.66	0.42
1:Y:52:TRP:HH2	1:Y:170:LEU:HD13	1.85	0.42
1:Y:338:VAL:O	1:Y:355:GLY:HA2	2.20	0.42
1:Y:380:LEU:HD13	1:Y:477:TRP:HZ2	1.84	0.42
1:Y:447:ASP:CB	1:Y:450:GLU:H	2.33	0.42
1:O:75:ALA:HB2	1:O:442:VAL:HG21	2.02	0.42
1:O:131:ALA:H	1:O:351:GLN:HE22	1.68	0.42
1:O:408:PHE:CD2	1:O:408:PHE:C	2.98	0.42
1:O:188:ASN:HD22	1:O:188:ASN:C	2.27	0.42
1:O:376:ALA:O	1:O:380:LEU:HD22	2.19	0.42
1:O:459:ARG:HH11	1:O:459:ARG:HD3	1.68	0.42
1:O:222:THR:O	1:O:223:LYS:C	2.63	0.42
1:O:270:ASP:OD1	1:O:292:SER:OG	2.38	0.41
1:O:340:ALA:O	1:O:341:PHE:C	2.60	0.41
1:O:427:LYS:HA	1:O:427:LYS:HD3	1.67	0.41
1:O:114:LYS:HG3	1:O:129:PRO:HB2	2.02	0.41
1:Y:474:TYR:O	1:Y:478:LYS:HG3	2.20	0.41
1:Y:179:SER:CB	1:Y:241:GLN:HG3	2.50	0.41
1:Y:376:ALA:O	1:Y:380:LEU:HD22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:34:PHE:HA	1:O:35:PRO:HD3	1.85	0.41
1:O:356:ILE:HG22	1:Y:358:ILE:CG1	2.48	0.41
1:Y:188:ASN:HD22	1:Y:190:LYS:N	2.15	0.41
1:Y:79:THR:HG21	1:Y:242:ALA:CB	2.51	0.41
1:Y:139:LYS:O	1:Y:140:TRP:C	2.64	0.41
1:O:48:PRO:HD3	1:O:97:ASN:HA	2.03	0.41
1:O:242:ALA:O	1:O:433:GLY:HA3	2.21	0.41
1:O:202:PHE:HB2	1:O:204:ILE:CD1	2.50	0.41
1:O:374:LEU:HD23	1:O:374:LEU:HA	1.85	0.41
1:Y:43:TRP:CE2	1:Y:105:ARG:HB2	2.55	0.41
1:Y:258:THR:OG1	1:Y:400:ASP:OD2	2.32	0.41
1:Y:317:LYS:HB2	1:Y:317:LYS:HE2	1.88	0.40
1:O:261:THR:HG23	1:O:304:ALA:HB2	2.03	0.40
1:O:346:ALA:HA	1:O:347:PRO:HA	1.81	0.40
1:O:469:THR:O	1:O:470:ARG:C	2.64	0.40
1:Y:183:ARG:NH2	1:Y:296:GLU:OE1	2.55	0.40
1:Y:447:ASP:HB3	1:Y:450:GLU:H	1.86	0.40
1:O:36:GLN:OE1	1:O:46:HIS:CE1	2.70	0.40
1:O:268:ASN:OD1	1:O:270:ASP:HB3	2.21	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	O	492/497 (99%)	460 (94%)	31 (6%)	1 (0%)	43	58
1	Y	492/497 (99%)	463 (94%)	26 (5%)	3 (1%)	21	32
All	All	984/994 (99%)	923 (94%)	57 (6%)	4 (0%)	30	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	490	VAL
1	Y	114	LYS
1	Y	111	GLU
1	O	169	ARG

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	O	406/409 (99%)	349 (86%)	57 (14%)	3	4
1	Y	406/409 (99%)	341 (84%)	65 (16%)	2	3
All	All	812/818 (99%)	690 (85%)	122 (15%)	3	3

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	1	MET
1	O	10	GLU
1	O	16	ARG
1	O	19	ILE
1	O	47	ASN
1	O	56	LEU
1	O	57	ARG
1	O	64	GLN
1	O	67	ARG
1	O	81	GLN
1	O	86	LEU
1	O	90	LYS
1	O	91	ASP
1	O	109	MET
1	O	112	GLU
1	O	113	ILE
1	O	119	THR
1	O	120	MET
1	O	122	LYS
1	O	123	GLU

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Mol	Chain	Res	Type
1	O	125	THR
1	O	127	LEU
1	O	138	LEU
1	O	141	LEU
1	O	148	LEU
1	O	177	ASP
1	O	188	ASN
1	O	198	LEU
1	O	199	LEU
1	O	201	LEU
1	O	208	VAL
1	O	224	LYS
1	O	241	GLN
1	O	270	ASP
1	O	290	ARG
1	O	317	LYS
1	O	342	VAL
1	O	367	GLU
1	O	380	LEU
1	O	391	LEU
1	O	395	LYS
1	O	398	ARG
1	O	416	ILE
1	O	417	LEU
1	O	423	ARG
1	O	424	PRO
1	O	429	THR
1	O	432	LEU
1	O	437	LEU
1	O	440	LEU
1	O	453	GLU
1	O	462	GLU
1	O	464	LYS
1	O	468	LYS
1	O	472	ARG
1	O	475	LYS
1	O	490	VAL
1	Y	2	GLU
1	Y	6	LEU
1	Y	7	SER
1	Y	8	LEU
1	Y	10	GLU

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Mol	Chain	Res	Type
1	Y	14	SER
1	Y	18	ILE
1	Y	22	ARG
1	Y	26	ILE
1	Y	29	ILE
1	Y	47	ASN
1	Y	53	ASP
1	Y	64	GLN
1	Y	67	ARG
1	Y	79	THR
1	Y	90	LYS
1	Y	93	LYS
1	Y	99	ILE
1	Y	105	ARG
1	Y	112	GLU
1	Y	119	THR
1	Y	120	MET
1	Y	122	LYS
1	Y	125	THR
1	Y	138	LEU
1	Y	170	LEU
1	Y	171	THR
1	Y	188	ASN
1	Y	198	LEU
1	Y	199	LEU
1	Y	207	SER
1	Y	208	VAL
1	Y	213	ARG
1	Y	223	LYS
1	Y	226	LEU
1	Y	227	LEU
1	Y	230	GLU
1	Y	234	SER
1	Y	241	GLN
1	Y	267	VAL
1	Y	313	ILE
1	Y	330	GLU
1	Y	356	ILE
1	Y	362	ARG
1	Y	367	GLU
1	Y	380	LEU
1	Y	391	LEU

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Mol	Chain	Res	Type
1	Y	394	ILE
1	Y	398	ARG
1	Y	399	VAL
1	Y	416	ILE
1	Y	417	LEU
1	Y	429	THR
1	Y	432	LEU
1	Y	437	LEU
1	Y	440	LEU
1	Y	442	VAL
1	Y	443	ASP
1	Y	453	GLU
1	Y	454	LEU
1	Y	464	LYS
1	Y	468	LYS
1	Y	485	MET
1	Y	491	VAL
1	Y	493	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	37	HIS
1	O	46	HIS
1	O	47	ASN
1	O	64	GLN
1	O	72	GLN
1	O	80	ASN
1	O	81	GLN
1	O	144	ASN
1	O	174	HIS
1	O	180	ASN
1	O	188	ASN
1	O	278	ASN
1	O	307	GLN
1	O	351	GLN
1	O	413	GLN
1	O	418	ASN
1	Y	31	GLN
1	Y	37	HIS
1	Y	46	HIS
1	Y	47	ASN

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Mol	Chain	Res	Type
1	Y	55	GLN
1	Y	72	GLN
1	Y	80	ASN
1	Y	102	GLN
1	Y	144	ASN
1	Y	174	HIS
1	Y	180	ASN
1	Y	188	ASN
1	Y	318	HIS
1	Y	351	GLN
1	Y	413	GLN
1	Y	418	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	O	494/497 (99%)	-0.38	3 (0%) 85 83	24, 43, 68, 98	0
1	Y	494/497 (99%)	-0.36	3 (0%) 85 83	25, 46, 69, 99	0
All	All	988/994 (99%)	-0.37	6 (0%) 85 83	24, 45, 68, 99	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	494	ALA	5.5
1	O	491	VAL	4.1
1	O	493	SER	3.9
1	O	494	ALA	3.6
1	Y	493	SER	2.5
1	Y	491	VAL	2.4

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 oligosaccharides 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.