



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:42 AM UTC

PDB ID : 3H3D / pdb_00003h3d
Title : Drosophila Pumilio RNA binding domain (Puf domain)
Authors : Edwards, T.A.; Aggarwal, A.K.; Wharton, R.P.
Deposited on : 2009-04-16
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

<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

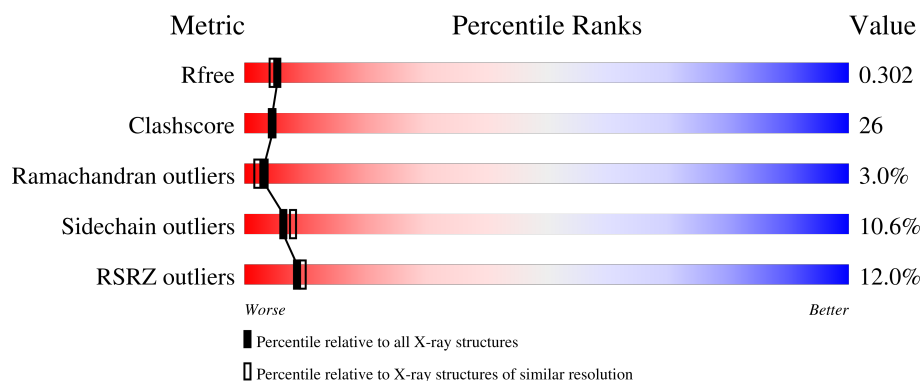
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	X	323	11% 47% 36% 10% • •
1	Y	323	13% 47% 38% 11% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5344 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 Maternal protein pumilio.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	313	Total	C	N	O	S	0	0	0
			2501	1577	438	469	17			
1	Y	314	Total	C	N	O	S	0	0	0
			2508	1581	442	468	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	GLY	-	expression tag	UNP P25822
X	-1	SER	-	expression tag	UNP P25822
X	0	HIS	-	expression tag	UNP P25822
X	1	MET	-	expression tag	UNP P25822
X	315	LYS	PRO	SEE REMARK 999	UNP P25822
X	316	ASN	HIS	SEE REMARK 999	UNP P25822
Y	312	GLY	-	expression tag	UNP P25822
Y	313	SER	-	expression tag	UNP P25822
Y	314	HIS	-	expression tag	UNP P25822
Y	315	MET	-	expression tag	UNP P25822
Y	629	LYS	PRO	SEE REMARK 999	UNP P25822
Y	630	ASN	HIS	SEE REMARK 999	UNP P25822

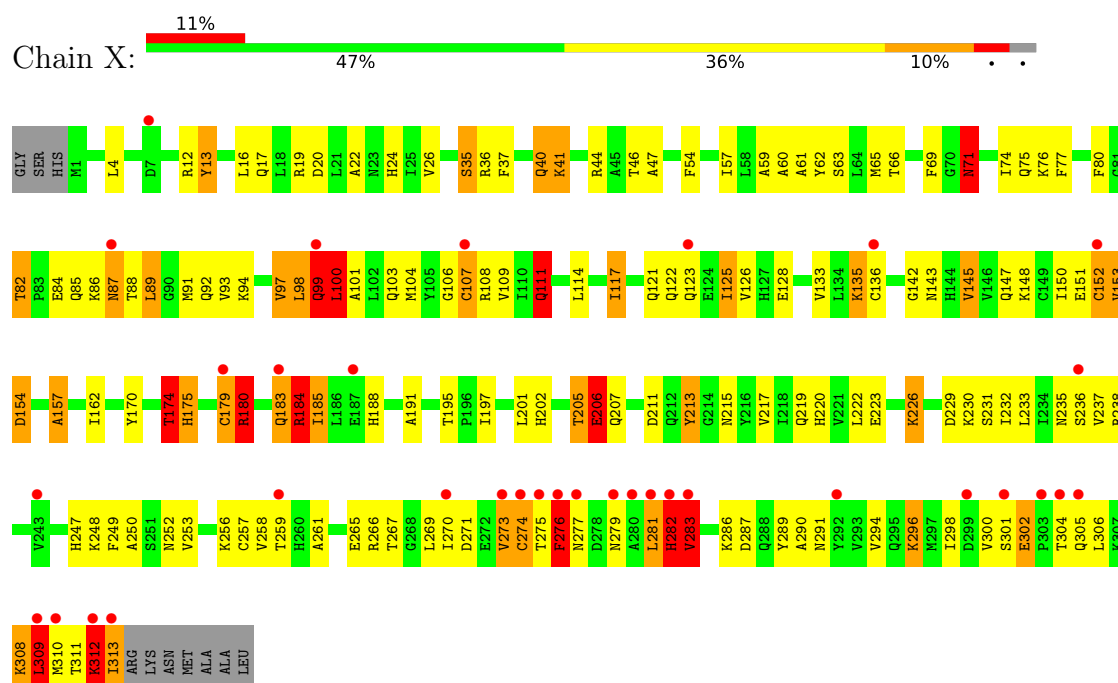
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	179	Total	O	0	0
			179	179		
2	Y	156	Total	O	0	0
			156	156		

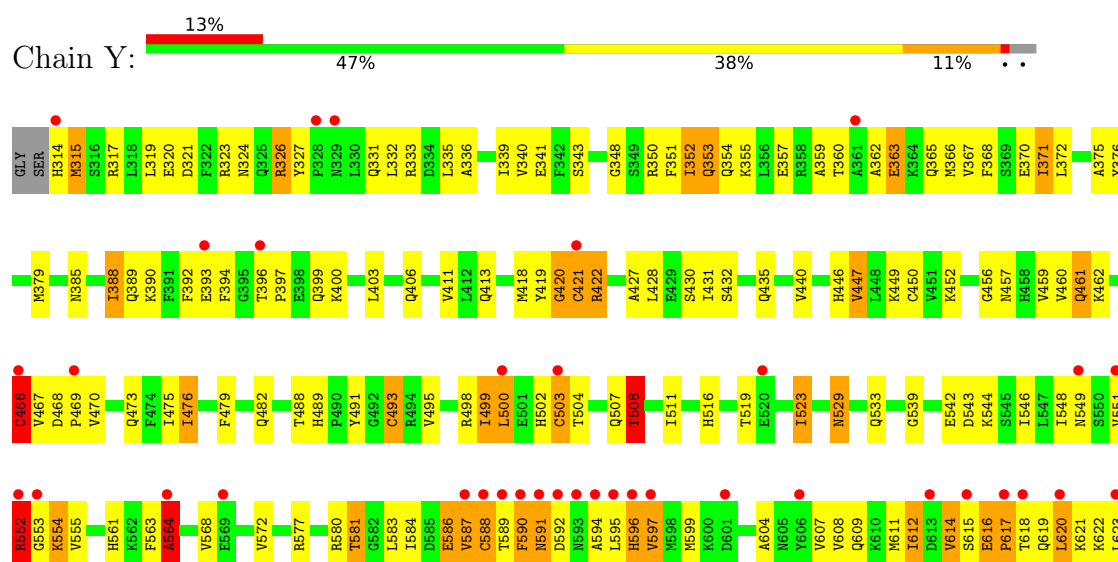
3 Residue-property plots

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: Maternal protein pumilio



• Molecule 1: Maternal protein pumilio



M624	T625	R626	T627	ARG	LYS	ASN	MET	ALA	ALA	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	94.58Å 94.58Å 229.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.78 – 2.30 19.78 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (19.78-2.30) 94.5 (19.78-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.252 , 0.298 0.252 , 0.302	Depositor DCC
R_{free} test set	2440 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.079 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5344	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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	X	1.90	45/2544 (1.8%)	1.68	53/3435 (1.5%)
1	Y	1.80	43/2551 (1.7%)	1.65	39/3444 (1.1%)
All	All	1.85	88/5095 (1.7%)	1.66	92/6879 (1.3%)

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	X	0	1

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	107	CYS	CA-CB	21.78	1.87	1.53
1	X	107	CYS	CB-SG	19.07	2.44	1.81
1	Y	421	CYS	CA-CB	18.90	1.85	1.53
1	Y	421	CYS	N-CA	18.71	1.70	1.46
1	X	183	GLN	CD-NE2	15.73	1.66	1.33
1	X	107	CYS	N-CA	10.33	1.58	1.46
1	X	302	GLU	CA-C	10.00	1.65	1.52
1	Y	466	CYS	CB-SG	9.67	2.13	1.81
1	X	111	GLN	CG-CD	9.44	1.75	1.52
1	X	57	ILE	CA-CB	-9.26	1.42	1.54
1	Y	420	GLY	C-N	9.19	1.46	1.33
1	X	300	VAL	CA-CB	8.73	1.64	1.54
1	X	183	GLN	CB-CG	8.38	1.77	1.52
1	X	183	GLN	CG-CD	8.35	1.73	1.52
1	Y	411	VAL	CA-CB	8.17	1.64	1.54
1	X	180	ARG	N-CA	7.98	1.56	1.46
1	X	107	CYS	C-O	-7.92	1.14	1.24
1	Y	461	GLN	C-O	7.41	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	466	CYS	CA-CB	7.38	1.65	1.53
1	Y	421	CYS	CA-C	7.33	1.62	1.52
1	X	136	CYS	C-O	-7.20	1.14	1.24
1	Y	614	VAL	CA-CB	7.18	1.62	1.54
1	X	60	ALA	CA-CB	7.01	1.62	1.53
1	X	74	ILE	CA-CB	7.00	1.62	1.54
1	Y	362	ALA	C-O	-6.87	1.16	1.24
1	X	302	GLU	N-CA	6.82	1.55	1.46
1	X	100	LEU	N-CA	6.80	1.54	1.46
1	Y	503	CYS	CB-SG	6.76	2.03	1.81
1	Y	427	ALA	CA-C	6.74	1.61	1.52
1	Y	422	ARG	N-CA	6.68	1.54	1.46
1	X	152	CYS	CB-SG	6.58	2.02	1.81
1	Y	421	CYS	CB-SG	6.55	2.02	1.81
1	X	213	TYR	CA-C	-6.50	1.45	1.52
1	X	98	LEU	C-O	-6.49	1.16	1.24
1	Y	459	VAL	CA-CB	6.40	1.62	1.54
1	X	205	THR	CA-C	-6.31	1.44	1.52
1	X	195	THR	CA-C	6.28	1.59	1.52
1	X	136	CYS	CB-SG	-6.22	1.60	1.81
1	Y	476	ILE	CA-CB	-6.12	1.47	1.54
1	X	114	LEU	C-O	-6.11	1.16	1.24
1	Y	482	GLN	C-O	-6.09	1.16	1.24
1	X	298	ILE	CA-CB	6.07	1.62	1.54
1	X	205	THR	CA-CB	-6.06	1.45	1.53
1	Y	367	VAL	CA-CB	-6.06	1.46	1.54
1	Y	393	GLU	CA-C	6.04	1.60	1.52
1	Y	456	GLY	C-O	-6.03	1.16	1.24
1	Y	588	CYS	N-CA	6.02	1.53	1.46
1	X	180	ARG	C-O	-5.81	1.16	1.24
1	Y	430	SER	N-CA	5.75	1.54	1.46
1	Y	588	CYS	CB-SG	5.70	2.00	1.81
1	Y	564	ALA	N-CA	5.70	1.53	1.46
1	Y	428	LEU	C-O	-5.69	1.17	1.24
1	Y	502	HIS	CA-C	-5.65	1.45	1.52
1	X	273	VAL	CA-C	5.64	1.59	1.52
1	Y	612	ILE	CA-CB	5.59	1.60	1.54
1	X	274	CYS	CB-SG	5.57	1.99	1.81
1	Y	446	HIS	N-CA	-5.54	1.40	1.46
1	Y	376	TYR	CA-C	-5.53	1.45	1.52
1	X	35	SER	C-O	-5.51	1.17	1.24
1	X	197	ILE	C-O	-5.50	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	372	LEU	N-CA	-5.48	1.39	1.46
1	X	253	VAL	CA-CB	5.45	1.61	1.54
1	Y	508	THR	CA-C	5.38	1.60	1.52
1	Y	352	ILE	CA-CB	-5.36	1.47	1.54
1	Y	495	VAL	CA-C	5.36	1.59	1.52
1	X	201	LEU	C-O	-5.35	1.17	1.24
1	Y	440	VAL	CA-CB	5.32	1.60	1.54
1	Y	564	ALA	CA-C	-5.31	1.45	1.52
1	X	206	GLU	CG-CD	5.30	1.65	1.52
1	Y	572	VAL	CA-CB	5.28	1.60	1.54
1	X	183	GLN	CA-C	5.26	1.59	1.52
1	X	44	ARG	CA-CB	5.26	1.60	1.53
1	X	26	VAL	C-O	-5.23	1.18	1.24
1	X	111	GLN	CA-CB	5.20	1.61	1.53
1	X	274	CYS	N-CA	5.19	1.52	1.46
1	Y	503	CYS	CA-C	5.19	1.59	1.52
1	X	142	GLY	C-O	-5.13	1.17	1.23
1	Y	488	THR	CA-C	5.10	1.60	1.52
1	X	157	ALA	CA-C	5.09	1.59	1.52
1	Y	584	ILE	CA-CB	5.09	1.60	1.54
1	X	256	LYS	C-O	-5.09	1.18	1.24
1	Y	447	VAL	CA-CB	5.06	1.60	1.54
1	Y	340	VAL	C-O	-5.05	1.18	1.24
1	X	276	PHE	N-CA	5.05	1.52	1.46
1	Y	352	ILE	C-O	-5.05	1.18	1.24
1	Y	351	PHE	CA-C	-5.03	1.46	1.52
1	X	99	GLN	CG-CD	5.03	1.64	1.52
1	X	71	ASN	CA-CB	5.02	1.61	1.53

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	421	CYS	N-CA-CB	17.44	139.96	110.49
1	Y	421	CYS	CA-CB-SG	15.27	149.53	114.40
1	X	107	CYS	CA-CB-SG	15.14	149.22	114.40
1	Y	420	GLY	CA-C-O	-14.71	104.12	120.30
1	X	107	CYS	N-CA-CB	13.71	130.66	109.82
1	Y	421	CYS	N-CA-C	-13.66	81.71	110.80
1	X	300	VAL	N-CA-C	9.60	121.26	112.43
1	X	152	CYS	N-CA-C	-9.26	95.78	110.14
1	X	136	CYS	CA-CB-SG	-8.94	93.84	114.40
1	Y	499	ILE	O-C-N	-8.80	114.90	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	422	ARG	N-CA-C	8.76	120.83	111.28
1	X	107	CYS	N-CA-C	-8.72	100.38	111.02
1	X	213	TYR	CA-C-N	-8.28	105.17	121.41
1	X	213	TYR	C-N-CA	-8.28	105.17	121.41
1	X	213	TYR	N-CA-C	-8.26	96.82	109.95
1	X	179	CYS	N-CA-C	-8.17	98.98	110.50
1	X	207	GLN	N-CA-C	-8.14	102.48	111.36
1	X	99	GLN	O-C-N	-7.95	112.87	122.65
1	X	13	TYR	CA-C-N	7.84	127.50	119.82
1	X	13	TYR	C-N-CA	7.84	127.50	119.82
1	X	97	VAL	CB-CA-C	-7.73	101.70	112.14
1	X	106	GLY	CA-C-O	-7.68	113.27	120.80
1	X	93	VAL	N-CA-C	-7.66	103.33	110.53
1	X	302	GLU	N-CA-C	7.65	126.71	109.81
1	Y	508	THR	N-CA-CB	-7.59	98.82	110.44
1	Y	352	ILE	N-CA-C	7.48	118.25	110.62
1	X	302	GLU	CA-C-N	-7.34	112.14	119.56
1	X	302	GLU	C-N-CA	-7.34	112.14	119.56
1	X	99	GLN	CA-C-N	-7.32	107.57	121.54
1	X	99	GLN	C-N-CA	-7.32	107.57	121.54
1	X	41	LYS	N-CA-C	7.17	120.14	111.82
1	X	133	VAL	N-CA-C	7.01	117.15	110.42
1	X	205	THR	CB-CA-C	-6.98	100.07	110.67
1	Y	420	GLY	CA-C-N	6.95	134.81	121.54
1	Y	420	GLY	C-N-CA	6.95	134.81	121.54
1	X	59	ALA	N-CA-C	6.84	119.58	111.71
1	Y	419	TYR	N-CA-C	-6.78	105.14	113.41
1	Y	420	GLY	O-C-N	6.77	129.66	122.28
1	X	175	HIS	N-CA-C	-6.68	100.06	110.14
1	X	145	VAL	N-CA-C	6.57	117.26	110.36
1	Y	341	GLU	N-CA-C	6.56	118.43	111.28
1	X	174	THR	N-CA-CB	-6.39	101.22	110.56
1	X	184	ARG	CB-CA-C	-6.35	100.91	110.88
1	X	106	GLY	CA-C-N	6.28	129.52	120.79
1	X	106	GLY	C-N-CA	6.28	129.52	120.79
1	Y	552	ARG	N-CA-C	6.26	124.13	110.80
1	X	183	GLN	N-CA-C	-6.25	104.55	111.36
1	X	183	GLN	CG-CD-OE1	-6.23	108.34	120.80
1	Y	462	LYS	N-CA-C	6.18	117.68	111.07
1	X	145	VAL	CG1-CB-CG2	5.99	123.98	110.80
1	Y	493	CYS	N-CA-C	5.90	118.47	111.33
1	X	180	ARG	N-CA-CB	5.90	120.46	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	108	ARG	N-CA-C	5.81	117.29	111.07
1	Y	549	ASN	N-CA-C	5.78	119.15	111.75
1	Y	459	VAL	CB-CA-C	-5.76	104.48	112.02
1	X	125	ILE	N-CA-C	5.67	115.86	110.53
1	X	13	TYR	N-CA-C	5.65	119.51	108.21
1	X	94	LYS	N-CA-C	5.64	118.15	111.33
1	X	183	GLN	CG-CD-NE2	5.62	124.83	116.40
1	Y	466	CYS	N-CA-CB	5.61	118.66	110.47
1	Y	315	MET	N-CA-C	5.59	122.70	110.80
1	Y	388	ILE	N-CA-C	-5.57	105.07	110.42
1	Y	503	CYS	CB-CA-C	5.55	119.67	109.46
1	X	273	VAL	CB-CA-C	5.53	119.00	111.87
1	Y	616	GLU	CA-C-N	5.53	126.75	119.84
1	Y	616	GLU	C-N-CA	5.53	126.75	119.84
1	Y	587	VAL	CB-CA-C	5.52	119.22	111.94
1	X	162	ILE	N-CA-C	-5.51	104.33	110.62
1	X	183	GLN	CB-CA-C	5.48	120.16	110.85
1	Y	614	VAL	CB-CA-C	5.45	118.30	111.65
1	X	145	VAL	N-CA-CB	5.44	116.55	110.51
1	X	220	HIS	N-CA-C	5.32	117.49	111.11
1	X	104	MET	N-CA-C	5.32	117.07	111.28
1	Y	626	LYS	N-CA-C	5.30	118.07	107.62
1	X	111	GLN	CB-CG-CD	5.27	121.56	112.60
1	Y	470	VAL	N-CA-C	5.26	118.43	111.17
1	Y	476	ILE	N-CA-C	5.18	115.80	110.36
1	X	135	LYS	CA-C-N	-5.18	111.88	120.68
1	X	135	LYS	C-N-CA	-5.18	111.88	120.68
1	Y	460	VAL	N-CA-CB	5.18	116.61	110.55
1	Y	604	ALA	CA-C-N	5.11	127.08	120.44
1	Y	604	ALA	C-N-CA	5.11	127.08	120.44
1	Y	353	GLN	N-CA-C	-5.08	104.82	111.02
1	Y	418	MET	N-CA-C	5.08	117.47	111.33
1	Y	467	VAL	CA-C-O	-5.07	117.68	121.68
1	Y	343	SER	CA-CB-OG	-5.05	101.00	111.10
1	X	205	THR	CA-C-N	-5.04	111.92	121.54
1	X	205	THR	C-N-CA	-5.04	111.92	121.54
1	Y	529	ASN	N-CA-C	-5.02	105.94	111.71
1	Y	508	THR	CA-C-N	5.02	126.98	120.26
1	Y	508	THR	C-N-CA	5.02	126.98	120.26
1	X	35	SER	CB-CA-C	-5.00	102.97	110.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	309	LEU	Peptide

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	X	2501	0	2491	120	0
1	Y	2508	0	2497	145	0
2	X	179	0	0	10	0
2	Y	156	0	0	12	0
All	All	5344	0	4988	260	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 26.

All (260) 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:X:111:GLN:CD	1:X:111:GLN:CG	1.75	1.58
1:X:183:GLN:CG	1:X:183:GLN:CB	1.77	1.56
1:Y:421:CYS:N	1:Y:421:CYS:CA	1.70	1.53
1:X:107:CYS:CA	1:X:107:CYS:CB	1.87	1.51
1:Y:421:CYS:CA	1:Y:421:CYS:CB	1.85	1.49
1:Y:421:CYS:CB	1:Y:421:CYS:SG	2.02	1.47
1:X:152:CYS:CB	1:X:152:CYS:SG	2.03	1.46
1:Y:503:CYS:CB	1:Y:503:CYS:SG	2.03	1.46
1:Y:466:CYS:CB	1:Y:466:CYS:SG	2.13	1.37
1:Y:317:ARG:HB2	2:Y:959:HOH:O	1.46	1.14
1:X:205:THR:O	1:X:206:GLU:HB2	1.34	1.11
1:X:312:LYS:H	1:X:312:LYS:HD2	1.15	1.11
1:Y:587:VAL:HG21	1:Y:611:MET:HE1	1.33	1.10
1:Y:431:ILE:HG21	1:Y:435:GLN:HE21	1.01	1.09
1:X:99:GLN:O	1:X:100:LEU:HB2	1.37	1.06
1:Y:499:ILE:O	1:Y:500:LEU:HB2	1.49	1.06
1:X:107:CYS:CB	1:X:107:CYS:SG	2.44	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:563:PHE:O	1:Y:564:ALA:CB	2.06	1.02
1:Y:421:CYS:N	1:Y:421:CYS:C	2.17	1.01
1:Y:431:ILE:CG2	1:Y:435:GLN:HE21	1.73	1.01
1:X:179:CYS:O	1:X:180:ARG:HB2	1.62	0.99
1:X:180:ARG:H	1:X:183:GLN:HG3	1.29	0.98
1:Y:620:LEU:O	1:Y:624:MET:HB2	1.64	0.98
1:Y:331:GLN:HB3	2:Y:894:HOH:O	1.65	0.95
1:X:99:GLN:O	1:X:100:LEU:CB	2.11	0.94
1:Y:616:GLU:O	1:Y:618:THR:N	2.00	0.93
1:X:215:ASN:HD22	1:X:219:GLN:HE21	1.16	0.93
1:X:107:CYS:CB	1:X:107:CYS:HA	1.99	0.92
1:X:205:THR:O	1:X:206:GLU:CB	2.13	0.92
1:Y:431:ILE:HG21	1:Y:435:GLN:NE2	1.84	0.91
1:X:312:LYS:HG3	2:Y:733:HOH:O	1.70	0.91
1:Y:615:SER:O	1:Y:616:GLU:HG2	1.74	0.88
1:Y:504:THR:H	1:Y:507:GLN:NE2	1.71	0.87
1:X:312:LYS:HD2	1:X:312:LYS:N	1.86	0.87
1:Y:563:PHE:O	1:Y:564:ALA:HB2	1.73	0.86
1:X:305:GLN:HE22	1:Y:620:LEU:HD23	1.41	0.84
1:X:281:LEU:O	1:X:282:HIS:C	2.18	0.84
1:Y:421:CYS:CB	1:Y:421:CYS:HA	2.08	0.84
1:Y:499:ILE:O	1:Y:500:LEU:CB	2.20	0.83
1:Y:590:PHE:CE1	1:Y:595:LEU:HD23	2.14	0.82
1:X:61:ALA:O	1:X:65:MET:HG3	1.78	0.82
1:Y:589:THR:O	1:Y:590:PHE:O	1.99	0.81
1:X:188:HIS:HD2	2:X:701:HOH:O	1.63	0.80
1:Y:577:ARG:O	1:Y:581:THR:HG23	1.82	0.80
1:Y:542:GLU:O	1:Y:546:ILE:HD12	1.82	0.78
1:X:222:LEU:O	1:X:230:LYS:HE2	1.83	0.78
1:Y:413:GLN:HG3	2:Y:1010:HOH:O	1.83	0.78
1:X:312:LYS:O	1:X:313:ILE:O	2.03	0.75
1:Y:396:THR:HG23	1:Y:399:GLN:H	1.52	0.75
1:X:215:ASN:HD22	1:X:219:GLN:NE2	1.85	0.74
1:X:215:ASN:ND2	1:X:219:GLN:HE21	1.84	0.74
1:Y:504:THR:H	1:Y:507:GLN:HE21	1.35	0.73
1:X:19:ARG:HD3	2:X:977:HOH:O	1.88	0.73
1:Y:616:GLU:HB3	1:Y:617:PRO:HD2	1.71	0.73
1:X:215:ASN:ND2	1:X:219:GLN:NE2	2.36	0.72
1:Y:319:LEU:O	1:Y:323:ARG:HG3	1.89	0.72
1:Y:348:GLY:O	1:Y:352:ILE:HG13	1.90	0.72
1:Y:590:PHE:HB2	1:Y:594:ALA:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:321:ASP:HB2	1:Y:327:TYR:HE1	1.55	0.70
1:Y:590:PHE:HE1	1:Y:595:LEU:HD23	1.57	0.70
1:X:143:ASN:O	1:X:147:GLN:HG3	1.92	0.69
1:X:191:ALA:HB2	1:X:226:LYS:HE3	1.75	0.69
1:X:152:CYS:O	1:X:153:VAL:HB	1.92	0.68
1:X:82:THR:HG22	1:X:85:GLN:H	1.59	0.68
1:X:305:GLN:NE2	1:Y:620:LEU:HD23	2.09	0.67
1:X:188:HIS:CD2	2:X:701:HOH:O	2.41	0.67
1:X:267:THR:O	1:X:271:ASP:HB2	1.95	0.67
1:Y:618:THR:HA	1:Y:621:LYS:HG2	1.77	0.67
1:Y:587:VAL:HG21	1:Y:611:MET:CE	2.21	0.67
1:Y:355:LYS:O	1:Y:359:ALA:HB2	1.95	0.66
1:Y:617:PRO:HD3	2:Y:848:HOH:O	1.96	0.66
1:X:183:GLN:HG2	1:X:217:VAL:HG22	1.78	0.66
1:X:54:PHE:HB2	1:X:77:PHE:CZ	2.30	0.66
1:Y:563:PHE:O	1:Y:564:ALA:HB3	1.92	0.66
1:X:103:GLN:HG3	2:X:869:HOH:O	1.95	0.66
1:Y:375:ALA:O	1:Y:379:MET:HG3	1.96	0.65
1:Y:475:ILE:HG22	1:Y:499:ILE:HD11	1.78	0.65
1:X:170:TYR:O	1:X:174:THR:HB	1.97	0.65
1:X:179:CYS:O	1:X:180:ARG:CB	2.36	0.65
1:Y:431:ILE:CG2	1:Y:435:GLN:NE2	2.51	0.64
1:Y:564:ALA:O	1:Y:568:VAL:HG23	1.96	0.64
1:Y:431:ILE:HG22	1:Y:432:SER:N	2.12	0.64
1:X:126:VAL:HG21	1:X:153:VAL:HG21	1.80	0.64
1:Y:561:HIS:CD2	1:Y:563:PHE:O	2.52	0.63
1:X:87:ASN:HA	1:X:121:GLN:HE22	1.64	0.63
1:Y:612:ILE:HG12	1:Y:623:LEU:HD11	1.80	0.62
1:X:36:ARG:NH2	2:X:1027:HOH:O	2.30	0.62
1:Y:595:LEU:HD13	1:Y:596:HIS:ND1	2.14	0.62
1:Y:396:THR:HG22	1:Y:399:GLN:CG	2.30	0.61
1:X:147:GLN:O	1:X:151:GLU:HG3	2.01	0.61
1:Y:473:GLN:NE2	2:Y:814:HOH:O	2.33	0.61
1:Y:620:LEU:HD13	1:Y:624:MET:SD	2.40	0.61
1:X:150:ILE:HD13	1:X:185:ILE:HG12	1.83	0.61
1:X:122:GLN:O	1:X:126:VAL:HG23	2.01	0.60
1:X:202:HIS:HD2	2:X:767:HOH:O	1.84	0.60
1:Y:498:ARG:HG2	1:Y:498:ARG:HH11	1.66	0.59
1:Y:504:THR:N	1:Y:507:GLN:HE21	1.99	0.59
1:Y:516:HIS:HE1	1:Y:543:ASP:OD1	1.85	0.59
1:X:270:ILE:HD13	1:X:304:THR:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:620:LEU:O	1:Y:624:MET:CB	2.47	0.58
1:Y:421:CYS:CB	1:Y:421:CYS:C	2.74	0.58
1:Y:561:HIS:HD2	1:Y:563:PHE:H	1.52	0.58
1:Y:626:LYS:HG3	1:Y:627:ILE:HG13	1.84	0.58
1:Y:335:LEU:O	1:Y:336:ALA:C	2.46	0.58
1:Y:421:CYS:CA	1:Y:421:CYS:HB2	2.22	0.57
1:Y:590:PHE:HD1	1:Y:591:ASN:O	1.87	0.57
1:X:180:ARG:N	1:X:183:GLN:HG3	2.12	0.57
1:Y:326:ARG:HD3	2:Y:945:HOH:O	2.05	0.56
1:X:4:LEU:HD12	1:X:4:LEU:O	2.06	0.56
1:Y:612:ILE:HG13	1:Y:622:LYS:NZ	2.21	0.56
1:X:111:GLN:CG	1:X:111:GLN:NE2	2.63	0.56
1:Y:420:GLY:C	1:Y:421:CYS:C	2.73	0.56
1:Y:489:HIS:O	1:Y:493:CYS:SG	2.55	0.55
1:X:273:VAL:O	1:X:275:THR:N	2.39	0.55
1:Y:621:LYS:HA	1:Y:624:MET:HE2	1.87	0.55
1:X:249:PHE:O	1:X:252:ASN:HB2	2.07	0.55
1:Y:498:ARG:HG2	1:Y:498:ARG:NH1	2.22	0.55
1:Y:504:THR:O	1:Y:508:THR:HB	2.07	0.55
1:Y:592:ASP:O	1:Y:595:LEU:HD12	2.07	0.54
1:Y:597:VAL:HG11	2:Y:932:HOH:O	2.07	0.54
1:X:309:LEU:HD13	1:Y:623:LEU:HD22	1.89	0.54
1:X:261:ALA:HB3	1:X:266:ARG:HG3	1.89	0.54
1:Y:561:HIS:HD2	1:Y:563:PHE:O	1.89	0.54
1:X:247:HIS:HD2	1:X:249:PHE:H	1.55	0.54
1:X:312:LYS:HB3	1:Y:609:GLN:HE22	1.73	0.54
1:Y:539:GLY:O	1:Y:544:LYS:HE3	2.08	0.54
1:X:309:LEU:O	1:X:312:LYS:HD3	2.07	0.54
1:X:35:SER:OG	1:X:69:PHE:HB3	2.09	0.53
1:X:184:ARG:NH1	2:X:1015:HOH:O	2.40	0.53
1:X:247:HIS:HB3	1:X:250:ALA:HB3	1.89	0.53
1:X:287:ASP:HB3	1:X:290:ALA:HB3	1.89	0.53
1:X:36:ARG:O	1:X:40:GLN:HG3	2.08	0.53
1:X:123:GLN:HG3	2:X:834:HOH:O	2.08	0.53
1:X:238:ARG:NH2	1:X:265:GLU:O	2.41	0.53
1:Y:615:SER:HB2	1:Y:619:GLN:HB2	1.91	0.53
1:Y:321:ASP:CB	1:Y:327:TYR:HE1	2.21	0.52
1:Y:468:ASP:O	1:Y:469:PRO:C	2.52	0.52
1:X:257:CYS:O	1:X:261:ALA:HB2	2.10	0.52
1:X:211:ASP:OD2	1:X:213:TYR:O	2.29	0.51
1:X:82:THR:HG23	1:X:84:GLU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:233:LEU:O	1:X:236:SER:HB3	2.10	0.51
1:X:152:CYS:SG	1:X:152:CYS:CA	2.95	0.51
1:Y:396:THR:OG1	1:Y:397:PRO:HD2	2.10	0.51
1:Y:529:ASN:O	1:Y:533:GLN:HG3	2.11	0.51
1:Y:332:LEU:O	1:Y:366:MET:HE1	2.10	0.51
1:X:148:LYS:O	1:X:152:CYS:SG	2.69	0.51
1:X:191:ALA:CB	1:X:226:LYS:HE3	2.40	0.51
1:X:154:ASP:O	1:X:157:ALA:N	2.43	0.51
1:Y:363:GLU:O	1:Y:366:MET:HB3	2.11	0.50
1:Y:561:HIS:CD2	1:Y:563:PHE:H	2.30	0.50
1:Y:587:VAL:C	1:Y:588:CYS:O	2.51	0.50
1:Y:360:THR:OG1	1:Y:363:GLU:HG3	2.11	0.50
1:Y:421:CYS:N	1:Y:422:ARG:N	2.59	0.50
1:X:312:LYS:C	1:X:313:ILE:O	2.55	0.50
1:Y:390:LYS:HE3	1:Y:394:PHE:HE1	1.77	0.50
1:X:222:LEU:O	1:X:230:LYS:CE	2.56	0.50
1:Y:339:ILE:HB	1:Y:370:GLU:OE2	2.11	0.50
1:Y:592:ASP:OD1	1:Y:592:ASP:C	2.54	0.50
1:Y:392:PHE:O	1:Y:400:LYS:HE2	2.12	0.49
1:Y:375:ALA:HB1	1:Y:379:MET:HE3	1.93	0.49
1:X:12:ARG:HD3	1:X:13:TYR:CZ	2.48	0.49
1:Y:371:ILE:HD12	1:Y:388:ILE:HD13	1.93	0.49
1:X:247:HIS:CD2	1:X:249:PHE:H	2.30	0.49
1:Y:551:VAL:O	1:Y:554:LYS:HB2	2.13	0.49
1:X:46:THR:HG22	1:X:47:ALA:N	2.28	0.49
1:Y:396:THR:HG22	1:Y:399:GLN:HG3	1.95	0.49
1:X:117:ILE:HB	1:X:121:GLN:HE21	1.78	0.48
1:X:62:TYR:HA	1:X:65:MET:HE3	1.95	0.48
1:X:231:SER:O	1:X:235:ASN:HB3	2.13	0.48
1:Y:561:HIS:HE1	2:Y:774:HOH:O	1.95	0.48
1:X:17:GLN:HA	1:X:17:GLN:OE1	2.13	0.48
1:X:276:PHE:HD1	1:X:279:ASN:OD1	1.96	0.48
1:Y:396:THR:CG2	1:Y:399:GLN:H	2.24	0.48
1:X:66:THR:CG2	1:X:100:LEU:HD23	2.44	0.48
1:Y:499:ILE:HG21	1:Y:511:ILE:CD1	2.44	0.48
1:X:312:LYS:N	1:X:312:LYS:CD	2.68	0.48
1:Y:580:ARG:HD3	1:Y:614:VAL:HG12	1.96	0.48
1:X:259:THR:OG1	1:X:296:LYS:HE2	2.14	0.48
1:Y:529:ASN:OD1	1:Y:533:GLN:NE2	2.46	0.47
1:Y:625:THR:OG1	1:Y:625:THR:O	2.31	0.47
1:X:281:LEU:O	1:X:283:VAL:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:314:HIS:N	2:Y:883:HOH:O	2.47	0.47
1:X:82:THR:O	1:X:86:LYS:HG3	2.14	0.47
1:Y:612:ILE:HG12	1:Y:623:LEU:CD1	2.44	0.47
1:Y:607:VAL:HG12	1:Y:611:MET:HE2	1.96	0.47
1:X:62:TYR:OH	1:X:99:GLN:HG3	2.14	0.47
1:X:247:HIS:CD2	1:X:250:ALA:H	2.33	0.47
1:Y:616:GLU:C	1:Y:618:THR:H	2.15	0.47
1:Y:385:ASN:O	1:Y:389:GLN:HG3	2.15	0.47
1:X:202:HIS:HE1	1:X:229:ASP:OD1	1.98	0.47
1:Y:363:GLU:O	1:Y:366:MET:N	2.48	0.47
1:Y:544:LYS:O	1:Y:548:ILE:HD12	2.14	0.47
1:X:308:LYS:HB3	1:X:308:LYS:HE2	1.36	0.46
1:Y:616:GLU:O	1:Y:619:GLN:N	2.43	0.46
1:Y:431:ILE:HG22	1:Y:432:SER:H	1.78	0.46
1:Y:577:ARG:O	1:Y:581:THR:CG2	2.59	0.46
1:Y:475:ILE:CG2	1:Y:499:ILE:HD11	2.44	0.46
1:Y:354:GLN:NE2	2:Y:1000:HOH:O	2.49	0.46
1:X:247:HIS:HD2	1:X:250:ALA:H	1.64	0.46
1:Y:392:PHE:HE2	1:Y:431:ILE:HD11	1.80	0.46
1:X:22:ALA:O	1:X:24:HIS:HD2	1.99	0.46
1:X:175:HIS:O	1:X:179:CYS:SG	2.70	0.45
1:Y:333:ARG:HA	1:Y:366:MET:CE	2.46	0.45
1:X:296:LYS:HD3	1:X:296:LYS:HA	1.81	0.45
1:X:282:HIS:O	1:X:286:LYS:HB2	2.16	0.45
1:X:76:LYS:HE2	1:X:80:PHE:HE1	1.81	0.45
1:X:309:LEU:CD1	1:Y:623:LEU:HD22	2.47	0.45
1:Y:590:PHE:HB2	1:Y:594:ALA:CB	2.45	0.44
1:X:71:ASN:HD22	1:X:75:GLN:HE21	1.63	0.44
1:Y:519:THR:O	1:Y:523:ILE:HG23	2.17	0.44
1:X:87:ASN:CG	1:X:121:GLN:NE2	2.76	0.44
1:Y:479:PHE:CE1	1:Y:499:ILE:HD12	2.52	0.44
1:Y:457:ASN:O	1:Y:461:GLN:HG3	2.18	0.44
1:Y:587:VAL:O	1:Y:590:PHE:HB3	2.17	0.44
1:Y:392:PHE:CE2	1:Y:431:ILE:HD11	2.52	0.43
1:Y:608:VAL:HA	1:Y:611:MET:HE3	1.99	0.43
1:X:306:LEU:CD1	2:X:994:HOH:O	2.66	0.43
1:Y:400:LYS:O	1:Y:431:ILE:CD1	2.66	0.43
1:X:273:VAL:C	1:X:275:THR:H	2.27	0.43
1:Y:616:GLU:C	1:Y:618:THR:N	2.74	0.43
1:Y:618:THR:O	1:Y:622:LYS:HB3	2.18	0.43
1:X:308:LYS:C	1:X:310:MET:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:310:MET:HE3	1:X:310:MET:HA	1.99	0.43
1:Y:368:PHE:HE1	1:Y:403:LEU:HG	1.84	0.43
1:X:99:GLN:O	1:X:101:ALA:N	2.52	0.43
1:Y:333:ARG:HA	1:Y:366:MET:HE3	2.01	0.42
1:Y:561:HIS:HB3	1:Y:564:ALA:HB3	2.01	0.42
1:Y:392:PHE:CZ	1:Y:403:LEU:HB3	2.54	0.42
1:Y:612:ILE:HG13	1:Y:622:LYS:HZ1	1.84	0.42
1:X:65:MET:HB3	1:X:109:VAL:HG21	2.00	0.42
1:Y:355:LYS:HD2	2:Y:823:HOH:O	2.18	0.42
1:X:125:ILE:O	1:X:128:GLU:HB2	2.19	0.42
1:X:71:ASN:O	1:X:75:GLN:HG3	2.19	0.42
1:Y:595:LEU:O	1:Y:596:HIS:HB2	2.19	0.42
1:Y:403:LEU:O	1:Y:406:GLN:HB2	2.19	0.42
1:Y:431:ILE:CG2	1:Y:432:SER:N	2.81	0.42
1:X:87:ASN:CG	1:X:121:GLN:HE22	2.28	0.42
1:Y:552:ARG:HB3	1:Y:553:GLY:H	1.43	0.42
1:X:266:ARG:O	1:X:270:ILE:HG22	2.19	0.42
1:Y:539:GLY:O	1:Y:544:LYS:CE	2.67	0.42
1:X:281:LEU:HB3	1:X:282:HIS:H	1.67	0.42
1:Y:321:ASP:CB	1:Y:327:TYR:CE1	3.01	0.42
1:Y:452:LYS:O	1:Y:491:TYR:HD1	2.03	0.41
1:X:76:LYS:HA	1:X:76:LYS:HD2	1.89	0.41
1:X:88:THR:HA	1:X:91:MET:HE2	2.01	0.41
1:Y:504:THR:OG1	1:Y:507:GLN:HG3	2.20	0.41
1:X:16:LEU:HD12	1:X:20:ASP:OD2	2.21	0.41
1:Y:499:ILE:HG21	1:Y:499:ILE:HD13	1.81	0.41
1:X:148:LYS:HG3	1:X:152:CYS:SG	2.61	0.41
1:Y:561:HIS:HD2	1:Y:563:PHE:N	2.17	0.41
1:X:37:PHE:CE1	1:X:41:LYS:HE2	2.55	0.41
1:X:89:LEU:O	1:X:92:GLN:HB2	2.20	0.41
1:X:248:LYS:HG3	1:X:289:TYR:CZ	2.55	0.41
1:Y:421:CYS:CA	1:Y:421:CYS:HB3	2.22	0.41
1:X:233:LEU:HD23	2:X:767:HOH:O	2.19	0.41
1:X:150:ILE:CD1	1:X:185:ILE:HG12	2.51	0.40
1:X:219:GLN:O	1:X:223:GLU:HG2	2.21	0.40
1:Y:324:ASN:HB2	1:Y:326:ARG:HD2	2.02	0.40
1:Y:555:VAL:HB	1:Y:586:GLU:HG2	2.02	0.40
1:Y:390:LYS:HE3	1:Y:394:PHE:CE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	X	311/323 (96%)	288 (93%)	12 (4%)	11 (4%)	3	1
1	Y	312/323 (97%)	282 (90%)	22 (7%)	8 (3%)	4	3
All	All	623/646 (96%)	570 (92%)	34 (6%)	19 (3%)	3	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	180	ARG
1	X	282	HIS
1	X	312	LYS
1	Y	590	PHE
1	Y	617	PRO
1	X	100	LEU
1	X	153	VAL
1	X	206	GLU
1	X	274	CYS
1	Y	500	LEU
1	Y	564	ALA
1	X	302	GLU
1	Y	315	MET
1	Y	596	HIS
1	X	309	LEU
1	Y	363	GLU
1	X	276	PHE
1	Y	552	ARG
1	X	283	VAL

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	X	279/289 (96%)	244 (88%)	35 (12%)	4	5
1	Y	279/289 (96%)	255 (91%)	24 (9%)	10	13
All	All	558/578 (96%)	499 (89%)	59 (11%)	6	8

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	40	GLN
1	X	63	SER
1	X	71	ASN
1	X	82	THR
1	X	87	ASN
1	X	89	LEU
1	X	97	VAL
1	X	98	LEU
1	X	99	GLN
1	X	111	GLN
1	X	117	ILE
1	X	135	LYS
1	X	145	VAL
1	X	154	ASP
1	X	174	THR
1	X	184	ARG
1	X	185	ILE
1	X	206	GLU
1	X	226	LYS
1	X	232	ILE
1	X	237	VAL
1	X	258	VAL
1	X	269	LEU
1	X	277	ASN
1	X	281	LEU
1	X	282	HIS
1	X	283	VAL
1	X	291	ASN
1	X	294	VAL
1	X	296	LYS
1	X	301	SER
1	X	308	LYS
1	X	311	THR

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Mol	Chain	Res	Type
1	X	312	LYS
1	X	313	ILE
1	Y	320	GLU
1	Y	326	ARG
1	Y	350	ARG
1	Y	353	GLN
1	Y	357	GLU
1	Y	365	GLN
1	Y	371	ILE
1	Y	447	VAL
1	Y	449	LYS
1	Y	450	CYS
1	Y	466	CYS
1	Y	476	ILE
1	Y	508	THR
1	Y	523	ILE
1	Y	552	ARG
1	Y	554	LYS
1	Y	581	THR
1	Y	583	LEU
1	Y	586	GLU
1	Y	591	ASN
1	Y	597	VAL
1	Y	599	MET
1	Y	620	LEU
1	Y	625	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	15	ASN
1	X	24	HIS
1	X	32	GLN
1	X	71	ASN
1	X	87	ASN
1	X	121	GLN
1	X	122	GLN
1	X	127	HIS
1	X	144	HIS
1	X	147	GLN
1	X	188	HIS
1	X	202	HIS

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Mol	Chain	Res	Type
1	X	207	GLN
1	X	215	ASN
1	X	219	GLN
1	X	220	HIS
1	X	224	HIS
1	X	247	HIS
1	X	305	GLN
1	Y	338	HIS
1	Y	389	GLN
1	Y	401	ASN
1	Y	435	GLN
1	Y	455	ASN
1	Y	461	GLN
1	Y	497	GLN
1	Y	507	GLN
1	Y	516	HIS
1	Y	524	GLN
1	Y	561	HIS
1	Y	591	ASN
1	Y	593	ASN
1	Y	609	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

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	X	313/323 (96%)	0.67	34 (10%)	10 12	17, 39, 70, 87	0
1	Y	314/323 (97%)	0.80	41 (13%)	7 8	19, 42, 73, 97	0
All	All	627/646 (97%)	0.74	75 (11%)	9 9	17, 41, 72, 97	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	281	LEU	7.0
1	Y	625	THR	6.7
1	Y	594	ALA	6.6
1	X	313	ILE	6.5
1	Y	627	ILE	6.4
1	Y	588	CYS	6.1
1	X	280	ALA	6.0
1	X	309	LEU	5.8
1	X	274	CYS	5.7
1	Y	590	PHE	5.4
1	X	282	HIS	5.4
1	Y	591	ASN	5.3
1	X	276	PHE	5.3
1	Y	595	LEU	4.9
1	X	152	CYS	4.8
1	Y	596	HIS	4.6
1	X	136	CYS	4.5
1	Y	626	LYS	4.5
1	Y	503	CYS	4.4
1	Y	618	THR	4.3
1	Y	593	ASN	4.2
1	X	107	CYS	4.2
1	X	277	ASN	4.1
1	X	304	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	X	303	PRO	4.1
1	Y	617	PRO	3.9
1	X	301	SER	3.8
1	Y	466	CYS	3.6
1	X	275	THR	3.4
1	Y	421	CYS	3.3
1	X	312	LYS	3.3
1	Y	592	ASP	3.2
1	Y	606	TYR	3.2
1	Y	623	LEU	3.2
1	X	183	GLN	3.1
1	Y	589	THR	3.1
1	Y	620	LEU	3.1
1	Y	624	MET	3.1
1	X	123	GLN	3.1
1	X	310	MET	3.1
1	X	273	VAL	3.1
1	Y	469	PRO	3.0
1	X	283	VAL	2.8
1	Y	613	ASP	2.8
1	Y	329	ASN	2.7
1	X	292	TYR	2.6
1	X	259	THR	2.6
1	Y	314	HIS	2.6
1	X	179	CYS	2.5
1	Y	393	GLU	2.5
1	Y	361	ALA	2.5
1	X	299	ASP	2.5
1	X	305	GLN	2.5
1	Y	396	THR	2.5
1	X	279	ASN	2.5
1	X	270	ILE	2.4
1	Y	615	SER	2.4
1	Y	587	VAL	2.4
1	Y	551	VAL	2.4
1	Y	520	GLU	2.4
1	Y	569	GLU	2.4
1	Y	328	PRO	2.3
1	Y	552	ARG	2.3
1	Y	597	VAL	2.3
1	Y	549	ASN	2.3
1	X	7	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	Y	553	GLY	2.2
1	X	236	SER	2.2
1	Y	601	ASP	2.2
1	Y	500	LEU	2.1
1	X	187	GLU	2.1
1	X	87	ASN	2.1
1	X	99	GLN	2.1
1	Y	564	ALA	2.0
1	X	243	VAL	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 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.