WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 07:30 pm GMT

PDB ID	:	3H3D
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
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 2.30 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	Percentile Ranks	Value
Rfree		0.302
Clashscore		25
Ramachandran outliers		3.0%
Sidechain outliers		8.4%
RSRZ outliers		7.7%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
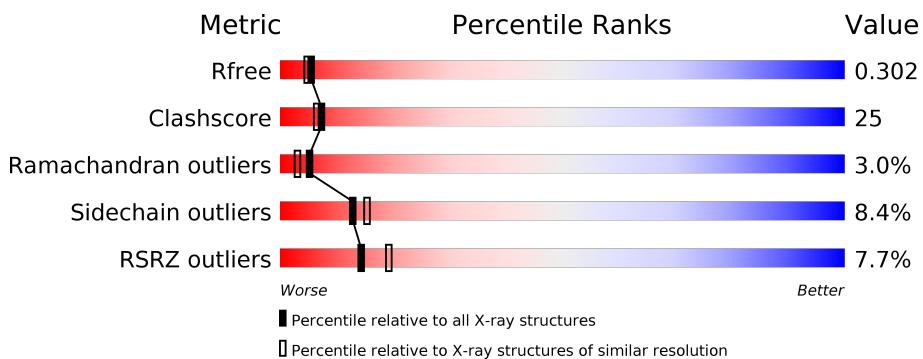
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	323	6% / 54% / 32% / 8% · ·
1	Y	323	9% / 56% / 34% / 6% · ·
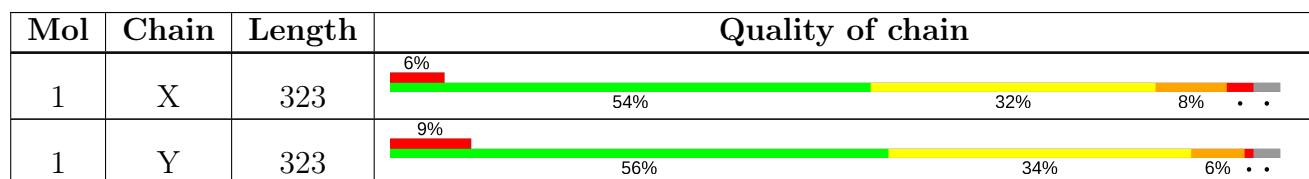
2 Entry composition ⓘ

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 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: Maternal protein pumilio
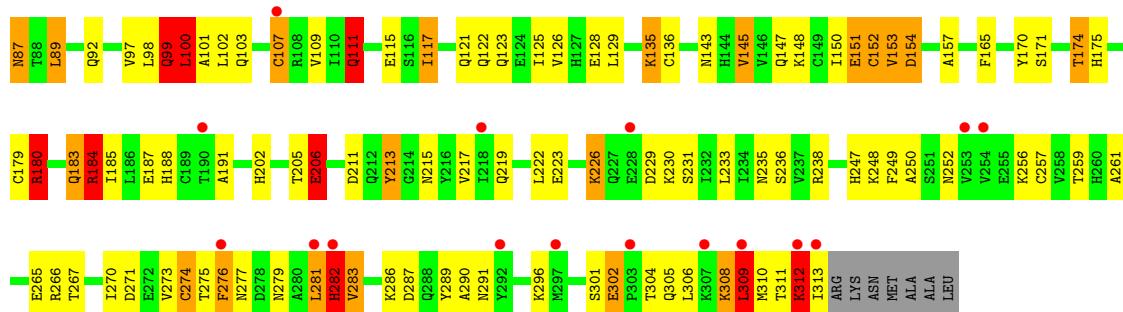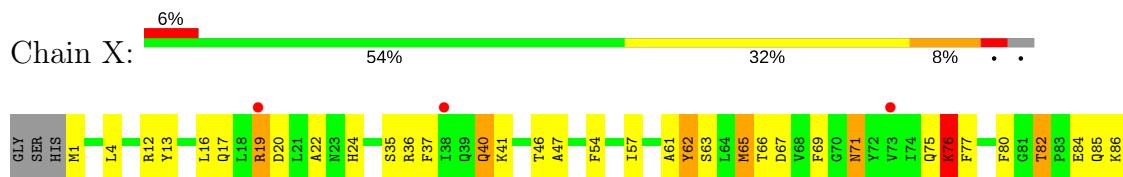
- Molecule 1: Maternal protein pumilio
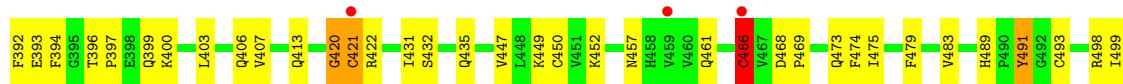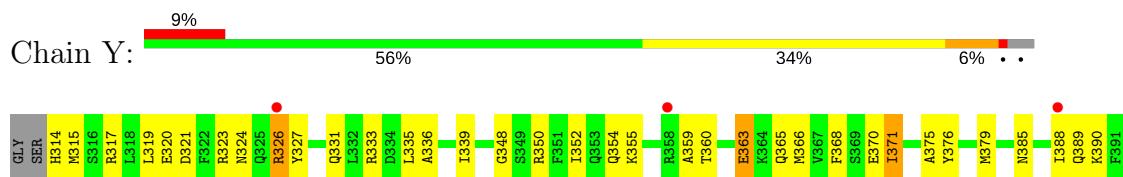
4 Data and refinement statistics (i)

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) 94.6 (19.78-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [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 (5.29%)	DCC
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 , 68.8	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.47, < L^2 > = 0.29$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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	1.68	22/2544 (0.9%)	1.28	25/3435 (0.7%)
1	Y	1.50	16/2551 (0.6%)	1.25	9/3444 (0.3%)
All	All	1.59	38/5095 (0.7%)	1.26	34/6879 (0.5%)

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 (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	107	CYS	CB-SG	36.44	2.44	1.82
1	Y	466	CYS	CB-SG	18.19	2.13	1.82
1	X	107	CYS	CA-CB	15.43	1.87	1.53
1	Y	421	CYS	CA-CB	14.30	1.85	1.53
1	X	183	GLN	CD-NE2	13.38	1.66	1.32
1	X	136	CYS	CB-SG	-12.67	1.60	1.82
1	Y	503	CYS	CB-SG	12.53	2.03	1.82
1	X	152	CYS	CB-SG	12.18	2.02	1.82
1	Y	421	CYS	CB-SG	12.13	2.02	1.82
1	Y	421	CYS	N-CA	11.99	1.70	1.46
1	X	111	GLN	CG-CD	10.69	1.75	1.51
1	Y	588	CYS	CB-SG	10.48	2.00	1.82
1	X	274	CYS	CB-SG	10.22	1.99	1.82
1	X	183	GLN	CG-CD	9.51	1.73	1.51
1	X	183	GLN	CB-CG	9.28	1.77	1.52
1	X	206	GLU	CG-CD	8.91	1.65	1.51
1	Y	376	TYR	CD2-CE2	8.65	1.52	1.39
1	X	97	VAL	CB-CG2	-7.34	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	206	GLU	CB-CG	6.60	1.64	1.52
1	X	115	GLU	CB-CG	-6.09	1.40	1.52
1	X	107	CYS	N-CA	5.97	1.58	1.46
1	Y	491	TYR	CD2-CE2	-5.90	1.30	1.39
1	X	99	GLN	CG-CD	5.90	1.64	1.51
1	X	165	PHE	CE1-CZ	5.68	1.48	1.37
1	Y	420	GLY	C-N	5.43	1.46	1.34
1	X	57	ILE	CA-CB	-5.39	1.42	1.54
1	X	62	TYR	CE2-CZ	5.38	1.45	1.38
1	Y	474	PHE	CE2-CZ	5.31	1.47	1.37
1	Y	491	TYR	CE2-CZ	-5.24	1.31	1.38
1	X	187	GLU	CB-CG	-5.16	1.42	1.52
1	Y	393	GLU	CB-CG	5.16	1.61	1.52
1	Y	535	VAL	CB-CG2	5.11	1.63	1.52
1	X	111	GLN	CB-CG	5.09	1.66	1.52
1	Y	407	VAL	CB-CG2	-5.08	1.42	1.52
1	Y	483	VAL	CB-CG1	5.07	1.63	1.52
1	X	180	ARG	N-CA	5.06	1.56	1.46
1	X	151	GLU	CB-CG	5.03	1.61	1.52
1	Y	466	CYS	CA-CB	5.02	1.65	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	421	CYS	CA-CB-SG	19.74	149.53	114.00
1	X	107	CYS	CA-CB-SG	19.57	149.22	114.00
1	Y	421	CYS	N-CA-CB	16.31	139.96	110.60
1	X	136	CYS	CA-CB-SG	-11.20	93.84	114.00
1	X	107	CYS	N-CA-CB	11.15	130.66	110.60
1	Y	421	CYS	N-CA-C	-10.85	81.71	111.00
1	Y	420	GLY	CA-C-O	-9.15	104.12	120.60
1	X	184	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	X	145	VAL	CG1-CB-CG2	8.18	123.98	110.90
1	X	213	TYR	C-N-CA	-8.15	105.17	122.30
1	X	100	LEU	CA-CB-CG	6.86	131.09	115.30
1	X	183	GLN	CG-CD-OE1	-6.63	108.34	121.60
1	X	76	LYS	CD-CE-NZ	-6.54	96.67	111.70
1	X	67	ASP	CB-CG-OD1	6.22	123.90	118.30
1	X	99	GLN	O-C-N	-6.14	112.87	122.70
1	Y	508	THR	N-CA-CB	-6.04	98.82	110.30
1	X	302	GLU	N-CA-C	5.82	126.71	111.00
1	X	184	ARG	NE-CZ-NH2	-5.73	117.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	99	GLN	C-N-CA	-5.65	107.57	121.70
1	X	152	CYS	N-CA-C	-5.63	95.78	111.00
1	Y	466	CYS	CA-CB-SG	5.57	124.03	114.00
1	X	180	ARG	N-CA-CB	5.48	120.46	110.60
1	X	19	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	Y	623	LEU	CA-CB-CG	-5.39	102.91	115.30
1	X	129	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	X	102	LEU	CB-CG-CD2	5.34	120.08	111.00
1	X	309	LEU	CA-CB-CG	-5.32	103.08	115.30
1	X	213	TYR	N-CA-C	-5.25	96.82	111.00
1	Y	583	LEU	CA-CB-CG	5.25	127.37	115.30
1	Y	420	GLY	C-N-CA	5.25	134.81	121.70
1	X	97	VAL	CB-CA-C	-5.11	101.70	111.40
1	X	65	MET	CG-SD-CE	5.10	108.35	100.20
1	X	1	MET	CB-CG-SD	5.07	127.61	112.40
1	X	135	LYS	CD-CE-NZ	-5.00	100.20	111.70

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 ⓘ

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	115	0
1	Y	2508	0	2497	139	0
2	X	179	0	0	10	0
2	Y	156	0	0	12	0
All	All	5344	0	4988	249	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 25.

All (249) 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:183:GLN:CB	1:X:183:GLN:CG	1.77	1.56
1:X:111:GLN:CG	1:X:111:GLN:CD	1.75	1.54
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:SG	1:X:152:CYS:CB	2.03	1.46
1:Y:503:CYS:SG	1:Y:503:CYS:CB	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:HD2	1:X:312:LYS:H	1.15	1.11
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
1:Y:563:PHE:O	1:Y:564:ALA:CB	2.06	1.02
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:421:CYS:N	1:Y:421:CYS:C	2.17	0.96
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:Y:421:CYS:HA	1:Y:421:CYS:CB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:281:LEU:O	1:X:282:HIS:C	2.18	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
1:Y:587:VAL:HG21	1:Y:611:MET:CE	2.21	0.71
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: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:587:VAL:HG21	1:Y:611:MET:HE1	1.78	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:Y:498:ARG:HG2	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
1:Y:620:LEU:O	1:Y:624:MET:CB	2.47	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: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: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:X:249:PHE:O	1:X:252:ASN:HB2	2.07	0.55
1:Y:498:ARG:NH1	1:Y:498:ARG:HG2	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:Y:539:GLY:O	1:Y:544:LYS:HE3	2.08	0.54
1:X:312:LYS:HB3	1:Y:609:GLN:HE22	1.73	0.54
1:X:309:LEU:O	1:X:312:LYS:HD3	2.07	0.54
1:X:184:ARG:NH1	2:X:1015:HOH:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:35:SER:OG	1:X:69:PHE:HB3	2.09	0.53
1:Y:421:CYS:C	1:Y:421:CYS:CB	2.74	0.53
1:Y:335:LEU:O	1:Y:336:ALA:C	2.46	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: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:233:LEU:O	1:X:236:SER:HB3	2.10	0.51
1:X:82:THR:HG23	1:X:84:GLU:H	1.75	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: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: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: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:392:PHE:O	1:Y:400:LYS:HE2	2.12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:499:ILE:HG21	1:Y:511:ILE:CD1	2.44	0.48
1:Y:587:VAL:C	1:Y:588:CYS:O	2.51	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:X:281:LEU:O	1:X:283:VAL:N	2.45	0.47
1:Y:625:THR:OG1	1:Y:625:THR:O	2.31	0.47
1:Y:314:HIS:N	2:Y:883:HOH:O	2.47	0.47
1:Y:468:ASP:O	1:Y:469:PRO:C	2.52	0.47
1:Y:612:ILE:HG13	1:Y:622:LYS:HZ1	1.79	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: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: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:HE2	1:X:308:LYS:HB3	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:HA	1:X:296:LYS:HD3	1.81	0.45
1:Y:333:ARG:HA	1:Y:366:MET:HE3	1.97	0.45
1:Y:592:ASP:C	1:Y:592:ASP:OD1	2.54	0.45
1:X:312:LYS:C	1:X:313:ILE:O	2.55	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:X:62:TYR:HA	1:X:65:MET:HE3	1.99	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:420:GLY:C	1:Y:421:CYS:C	2.73	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: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:Y:618:THR:O	1:Y:622:LYS:HB3	2.18	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: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: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:Y:616:GLU:C	1:Y:618:THR:H	2.15	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: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: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:X:223:GLU:OE2	1:X:256:LYS:NZ	2.49	0.41
1:Y:561:HIS:HD2	1:Y:563:PHE:N	2.17	0.41
1:X:248:LYS:HG3	1:X:289:TYR:CZ	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	X	311/323 (96%)	288 (93%)	12 (4%)	11 (4%)	4	2
1	Y	312/323 (97%)	282 (90%)	22 (7%)	8 (3%)	6	4
All	All	623/646 (96%)	570 (92%)	34 (6%)	19 (3%)	5	3

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

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Mol	Chain	Res	Type
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%)	251 (90%)	28 (10%)	9	10
1	Y	279/289 (96%)	260 (93%)	19 (7%)	18	24
All	All	558/578 (96%)	511 (92%)	47 (8%)	13	15

All (47) 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	76	LYS
1	X	82	THR
1	X	87	ASN
1	X	89	LEU
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	171	SER
1	X	174	THR
1	X	184	ARG
1	X	206	GLU
1	X	226	LYS
1	X	277	ASN

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Mol	Chain	Res	Type
1	X	281	LEU
1	X	282	HIS
1	X	291	ASN
1	X	301	SER
1	X	308	LYS
1	X	310	MET
1	X	311	THR
1	X	312	LYS
1	Y	320	GLU
1	Y	326	ARG
1	Y	350	ARG
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	508	THR
1	Y	523	ILE
1	Y	552	ARG
1	Y	581	THR
1	Y	583	LEU
1	Y	586	GLU
1	Y	591	ASN
1	Y	593	ASN
1	Y	599	MET
1	Y	625	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	24	HIS
1	X	32	GLN
1	X	39	GLN
1	X	71	ASN
1	X	87	ASN
1	X	121	GLN
1	X	122	GLN
1	X	144	HIS
1	X	188	HIS
1	X	202	HIS
1	X	215	ASN

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Mol	Chain	Res	Type
1	X	219	GLN
1	X	220	HIS
1	X	224	HIS
1	X	247	HIS
1	X	291	ASN
1	X	305	GLN
1	Y	338	HIS
1	Y	353	GLN
1	Y	401	ASN
1	Y	435	GLN
1	Y	507	GLN
1	Y	516	HIS
1	Y	534	HIS
1	Y	561	HIS
1	Y	609	GLN

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	X	313/323 (96%)	0.42	19 (6%)	22	28	17, 39, 71, 87	0
1	Y	314/323 (97%)	0.48	29 (9%)	10	13	19, 42, 73, 97	0
All	All	627/646 (97%)	0.45	48 (7%)	14	19	17, 41, 72, 97	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	276	PHE	8.9
1	Y	593	ASN	8.0
1	Y	590	PHE	4.9
1	Y	624	MET	4.3
1	Y	577	ARG	4.1
1	X	281	LEU	4.1
1	X	107	CYS	4.1
1	X	282	HIS	3.8
1	Y	596	HIS	3.7
1	Y	421	CYS	3.6
1	X	309	LEU	3.5
1	Y	626	LYS	3.5
1	Y	503	CYS	3.5
1	X	292	TYR	3.4
1	X	303	PRO	3.3
1	X	313	ILE	3.1
1	Y	568	VAL	3.1
1	X	38	ILE	3.1
1	X	254	VAL	3.0
1	X	253	VAL	2.9
1	X	190	THR	2.9
1	Y	618	THR	2.9
1	Y	532	ILE	2.9
1	Y	578	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	Y	326	ARG	2.7
1	X	297	MET	2.7
1	Y	589	THR	2.5
1	X	218	ILE	2.5
1	Y	606	TYR	2.5
1	X	312	LYS	2.4
1	X	73	VAL	2.4
1	Y	592	ASP	2.3
1	Y	627	ILE	2.3
1	Y	600	LYS	2.2
1	Y	625	THR	2.2
1	Y	588	CYS	2.2
1	X	19	ARG	2.2
1	Y	620	LEU	2.1
1	Y	623	LEU	2.1
1	X	307	LYS	2.1
1	Y	388	ILE	2.1
1	X	228	GLU	2.1
1	Y	459	VAL	2.1
1	Y	358	ARG	2.1
1	Y	466	CYS	2.1
1	Y	567	VAL	2.1
1	Y	520	GLU	2.0
1	Y	569	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.