



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2021 – 07:50 PM EDT

PDB ID : 3JW0
Title : E2 Ubiquitin-HECT
Authors : Kamadurai, H.B.; Schulman, B.A.
Deposited on : 2009-09-17
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

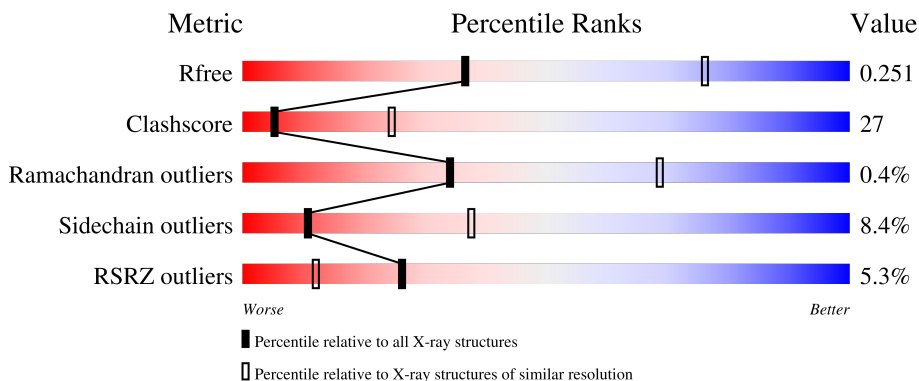
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 3.10 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	A	146	
1	B	146	
2	C	385	
2	D	385	
3	X	81	

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Mol	Chain	Length	Quality of chain
3	Y	81	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (31%), a green segment (46%), a yellow segment (46%), and a small grey segment (6%). The percentages are labeled below the bar.</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9826 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 Ubiquitin-conjugating enzyme E2 D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	146	1170	749	202	213	6	0	0	0
1	B	146	1170	749	202	213	6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	LEU	engineered mutation	UNP P62837
A	85	SER	CYS	engineered mutation	UNP P62837
A	98	LYS	THR	engineered mutation	UNP P62837
B	3	SER	LEU	engineered mutation	UNP P62837
B	85	SER	CYS	engineered mutation	UNP P62837
B	98	LYS	THR	engineered mutation	UNP P62837

- Molecule 2 is a protein called E3 ubiquitin-protein ligase NEDD4-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	376	3140	2032	519	572	17	0	0	0
2	D	374	3125	2021	517	570	17	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	571	GLY	-	expression tag	UNP Q96PU5
C	572	SER	-	expression tag	UNP Q96PU5
C	573	PRO	-	expression tag	UNP Q96PU5
C	574	GLU	-	expression tag	UNP Q96PU5
C	575	PHE	-	expression tag	UNP Q96PU5
C	922	SER	CYS	engineered mutation	UNP Q96PU5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	571	GLY	-	expression tag	UNP Q96PU5
D	572	SER	-	expression tag	UNP Q96PU5
D	573	PRO	-	expression tag	UNP Q96PU5
D	574	GLU	-	expression tag	UNP Q96PU5
D	575	PHE	-	expression tag	UNP Q96PU5
D	922	SER	CYS	engineered mutation	UNP Q96PU5

- Molecule 3 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
3	Y	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-4	GLY	-	expression tag	UNP P62988
X	-3	SER	-	expression tag	UNP P62988
X	-2	GLY	-	expression tag	UNP P62988
X	-1	GLY	-	expression tag	UNP P62988
X	0	SER	-	expression tag	UNP P62988
Y	-4	GLY	-	expression tag	UNP P62988
Y	-3	SER	-	expression tag	UNP P62988
Y	-2	GLY	-	expression tag	UNP P62988
Y	-1	GLY	-	expression tag	UNP P62988
Y	0	SER	-	expression tag	UNP P62988

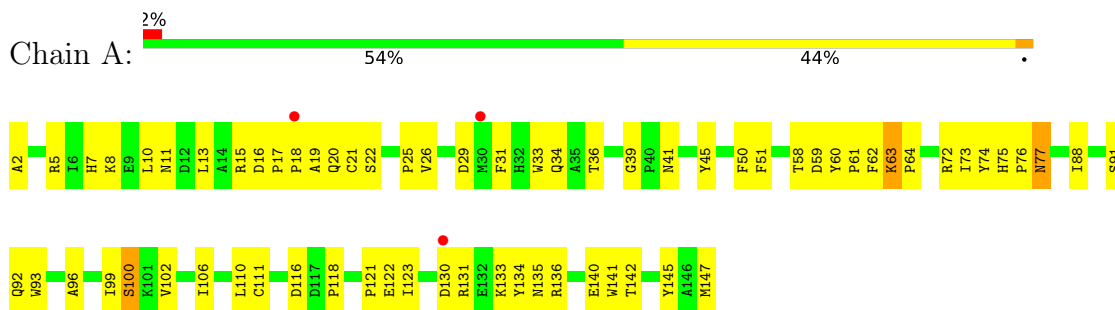
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	C	6	Total	O	0	0
			6	6		
4	D	11	Total	O	0	0
			11	11		
4	Y	1	Total	O	0	0
			1	1		

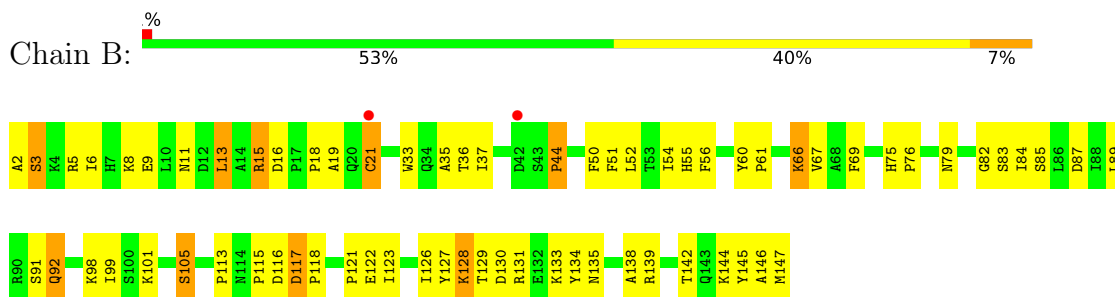
3 Residue-property plots [i](#)

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.

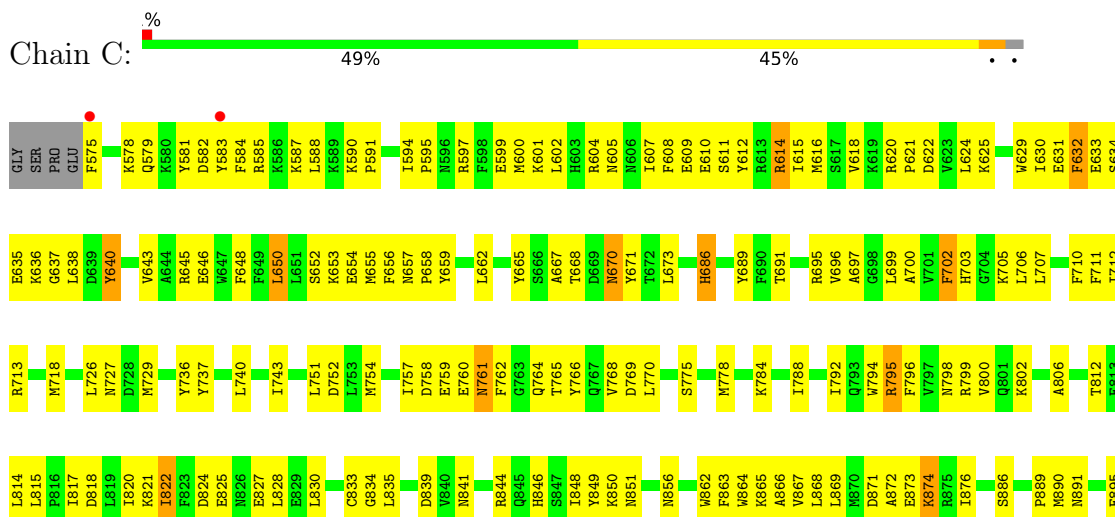
- Molecule 1: Ubiquitin-conjugating enzyme E2 D2



- Molecule 1: Ubiquitin-conjugating enzyme E2 D2

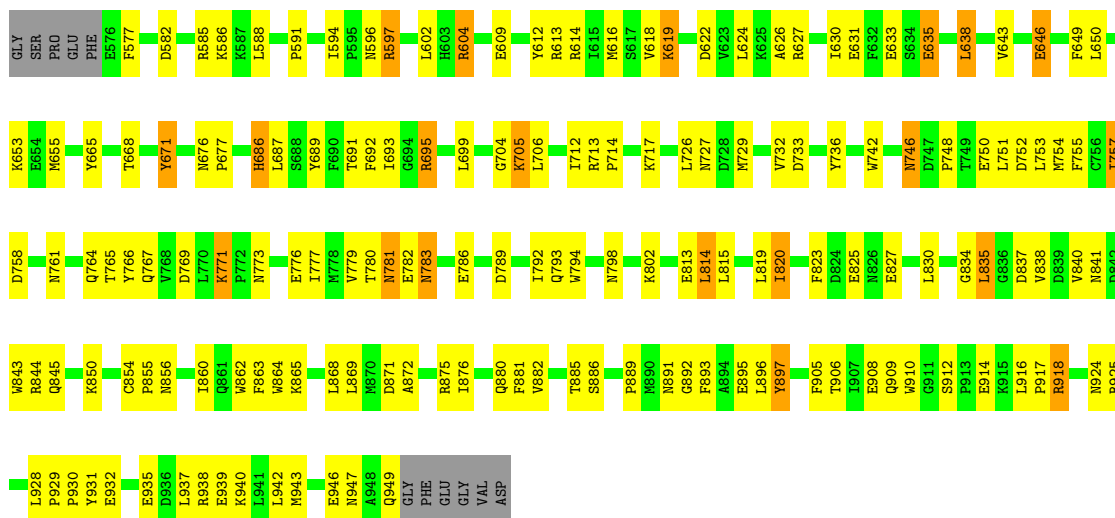


- Molecule 2: E3 ubiquitin-protein ligase NEDD4-like

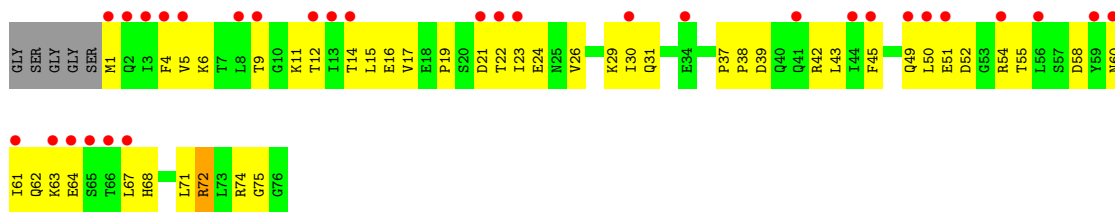




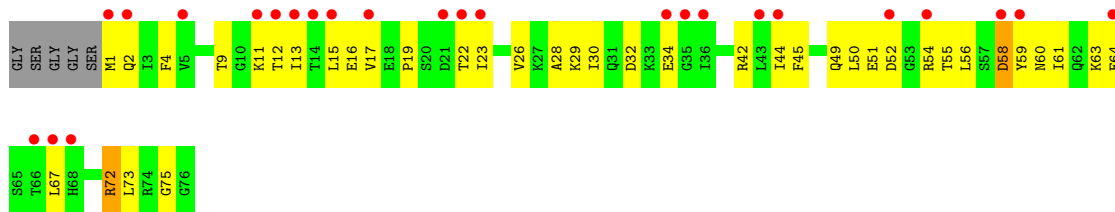
● Molecule 2: E3 ubiquitin-protein ligase NEDD4-like



● Molecule 3: Ubiquitin



● Molecule 3: Ubiquitin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.17Å 200.57Å 109.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.72 – 3.12	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 97.5 (49.72-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.46 (at 3.12Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.252 , 0.287 0.253 , 0.251	Depositor DCC
R_{free} test set	1700 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	80.9	Xtrriage
Anisotropy	0.247	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9826	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/1206	0.70	0/1642
1	B	0.41	0/1206	0.66	0/1642
2	C	0.47	0/3224	0.68	0/4355
2	D	0.49	0/3208	0.71	0/4334
3	X	0.44	0/607	0.68	0/816
3	Y	0.38	0/607	0.61	0/816
All	All	0.46	0/10058	0.69	0/13605

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1170	0	1152	73	0
1	B	1170	0	1152	62	0
2	C	3140	0	3057	171	0
2	D	3125	0	3045	163	0
3	X	601	0	629	45	0
3	Y	601	0	629	31	0
4	B	1	0	0	0	0
4	C	6	0	0	1	0
4	D	11	0	0	2	0
4	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9826	0	9664	518	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 27.

All (518) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:CE2	2:D:868:LEU:HD11	1.78	1.17
3:X:4:PHE:CD1	3:X:14:THR:HG22	1.95	1.01
2:C:906:THR:HB	2:C:925:ARG:HG3	1.47	0.96
2:D:733:ASP:OD2	2:D:736:TYR:HB2	1.69	0.93
1:B:116:ASP:O	1:B:118:PRO:HD3	1.69	0.92
2:C:630:ILE:O	2:C:643:VAL:HG21	1.70	0.92
2:C:933:THR:OG1	2:C:936:ASP:HB2	1.70	0.92
2:C:817:ILE:O	2:C:820:ILE:HG22	1.69	0.92
2:D:619:LYS:HE3	2:D:619:LYS:H	1.33	0.91
2:C:910:TRP:CH2	2:C:918:ARG:HD2	2.08	0.87
3:X:4:PHE:CE1	3:X:14:THR:HG22	2.10	0.86
2:C:848:ILE:HG13	2:C:906:THR:HG23	1.58	0.84
2:C:757:ILE:HG22	2:C:758:ASP:H	1.44	0.82
1:A:75:HIS:HE1	1:A:77:ASN:OD1	1.61	0.82
2:D:753:LEU:HB2	2:D:779:VAL:HG21	1.60	0.81
3:Y:26:VAL:O	3:Y:30:ILE:HG13	1.79	0.81
2:C:757:ILE:HD11	2:C:770:LEU:HD21	1.63	0.81
1:B:98:LYS:HG3	1:B:101:LYS:HE3	1.63	0.81
2:D:646:GLU:HG3	2:D:650:LEU:CD1	2.12	0.80
2:D:813:GLU:HB3	2:D:814:LEU:HD12	1.63	0.80
2:D:619:LYS:HE3	2:D:619:LYS:N	1.97	0.80
2:C:729:MET:HE1	2:C:740:LEU:HD12	1.62	0.79
1:B:116:ASP:O	1:B:118:PRO:CD	2.31	0.79
3:X:4:PHE:HD1	3:X:14:THR:HG22	1.47	0.78
2:C:944:ALA:O	2:C:948:ALA:HB2	1.84	0.78
2:C:876:ILE:HG22	2:C:886:SER:HB2	1.66	0.77
2:C:820:ILE:HD11	2:C:828:LEU:HD13	1.66	0.77
1:B:2:ALA:N	1:B:5:ARG:HB3	2.00	0.77
3:X:24:GLU:HB2	3:X:52:ASP:HB3	1.67	0.77
2:C:935:GLU:O	2:C:939:GLU:HG3	1.86	0.76
2:D:604:ARG:CG	2:D:604:ARG:HH11	1.99	0.76
2:D:910:TRP:CZ3	2:D:918:ARG:HD2	2.20	0.76
2:D:713:ARG:HB3	2:D:714:PRO:HD3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:O	1:A:140:GLU:HG3	1.83	0.76
1:B:131:ARG:HG3	1:B:135:ASN:HD21	1.49	0.76
1:A:26:VAL:HG13	2:D:871:ASP:HA	1.68	0.75
2:D:862:TRP:HB3	2:D:937:LEU:HD22	1.68	0.74
1:A:58:THR:HG21	2:C:760:GLU:HG3	1.69	0.74
2:D:918:ARG:HH12	3:Y:75:GLY:HA2	1.52	0.74
2:C:754:MET:HE2	2:C:778:MET:HG2	1.71	0.73
1:B:121:PRO:HG2	1:B:122:GLU:H	1.54	0.72
2:C:671:TYR:CE2	2:C:889:PRO:HG3	2.23	0.72
2:D:793:GLN:HG2	2:D:798:ASN:OD1	1.90	0.72
2:D:943:MET:O	2:D:947:ASN:ND2	2.22	0.71
3:X:45:PHE:HB3	3:X:50:LEU:HD21	1.72	0.71
1:A:75:HIS:CE1	1:A:77:ASN:OD1	2.43	0.71
2:D:837:ASP:OD1	2:D:872:ALA:HB1	1.90	0.71
1:A:13:LEU:O	1:A:17:PRO:HG3	1.91	0.70
2:D:780:THR:OG1	2:D:782:GLU:HG2	1.91	0.70
2:C:943:MET:CE	2:C:947:ASN:OD1	2.39	0.70
2:D:753:LEU:HB2	2:D:779:VAL:CG2	2.21	0.70
2:C:849:TYR:HE1	2:C:907:ILE:HD12	1.55	0.70
2:D:882:VAL:HG11	2:D:905:PHE:CE1	2.27	0.69
3:X:63:LYS:HE3	3:X:64:GLU:OE1	1.92	0.69
2:C:637:GLY:O	2:C:640:TYR:HE2	1.74	0.69
2:C:794:TRP:HA	2:C:798:ASN:HD22	1.57	0.69
2:C:729:MET:O	2:C:737:TYR:HB2	1.93	0.69
1:B:19:ALA:O	1:B:21:CYS:SG	2.51	0.68
2:D:638:LEU:CD2	2:D:638:LEU:H	2.07	0.68
2:C:656:PHE:HB3	2:C:673:LEU:HD13	1.75	0.68
2:D:794:TRP:HA	2:D:798:ASN:ND2	2.09	0.68
2:C:874:LYS:H	2:C:874:LYS:HD2	1.57	0.67
2:D:781:ASN:O	2:D:781:ASN:ND2	2.28	0.67
2:C:667:ALA:HB3	2:C:670:ASN:HB2	1.77	0.67
2:D:726:LEU:HA	2:D:792:ILE:HD13	1.77	0.67
2:C:602:LEU:HD22	2:C:610:GLU:HB3	1.77	0.67
3:X:1:MET:SD	3:X:19:PRO:HG3	2.35	0.66
3:Y:44:ILE:HD13	3:Y:49:GLN:HA	1.77	0.66
3:X:31:GLN:O	3:X:31:GLN:HG2	1.95	0.66
1:B:116:ASP:C	1:B:118:PRO:HD3	2.15	0.66
1:A:51:PHE:CE2	2:D:868:LEU:CD1	2.69	0.66
1:B:75:HIS:ND1	1:B:76:PRO:HD2	2.10	0.66
2:C:597:ARG:HD2	2:C:629:TRP:CE3	2.30	0.66
2:C:640:TYR:HD2	2:C:640:TYR:N	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:726:LEU:HA	2:C:792:ILE:CD1	2.26	0.65
2:C:640:TYR:N	2:C:640:TYR:CD2	2.64	0.65
2:D:896:LEU:HD23	2:D:897:TYR:N	2.11	0.65
2:D:830:LEU:HG	2:D:830:LEU:O	1.96	0.65
3:X:4:PHE:CE1	3:X:14:THR:CG2	2.81	0.64
3:Y:17:VAL:HG12	3:Y:29:LYS:NZ	2.11	0.64
1:A:72:ARG:HG3	1:A:72:ARG:HH11	1.61	0.64
2:C:726:LEU:HA	2:C:792:ILE:HD11	1.79	0.64
2:D:619:LYS:H	2:D:619:LYS:CE	2.10	0.64
2:D:704:GLY:O	2:D:705:LYS:HE2	1.97	0.64
2:D:862:TRP:O	2:D:865:LYS:HB3	1.97	0.64
2:C:601:LYS:HA	2:C:631:GLU:O	1.98	0.64
2:C:757:ILE:HG22	2:C:758:ASP:N	2.13	0.64
3:X:31:GLN:NE2	3:X:38:PRO:HD3	2.12	0.64
3:Y:2:GLN:H	3:Y:63:LYS:HD2	1.63	0.64
1:B:67:VAL:HG12	1:B:84:ILE:HD12	1.80	0.64
2:D:706:LEU:HD22	2:D:834:GLY:N	2.14	0.63
2:D:646:GLU:HG3	2:D:650:LEU:HD13	1.79	0.63
2:D:814:LEU:HD12	2:D:814:LEU:N	2.13	0.63
2:D:916:LEU:HD23	2:D:940:LYS:HG3	1.80	0.63
2:C:754:MET:CE	2:C:778:MET:HG2	2.28	0.63
3:X:42:ARG:HG3	3:X:72:ARG:HG2	1.80	0.63
1:A:36:THR:CG2	2:D:868:LEU:HD13	2.29	0.63
1:B:144:LYS:HD2	1:B:145:TYR:CZ	2.34	0.63
2:D:910:TRP:CH2	2:D:918:ARG:HD2	2.34	0.63
2:C:876:ILE:CG2	2:C:886:SER:HB2	2.29	0.63
2:C:581:TYR:O	2:C:584:PHE:HB3	1.98	0.62
3:Y:54:ARG:HD2	3:Y:58:ASP:HB3	1.82	0.62
1:B:55:HIS:HB3	1:B:66:LYS:HG3	1.80	0.62
2:C:918:ARG:O	2:C:926:LEU:HD12	2.01	0.61
2:D:638:LEU:H	2:D:638:LEU:HD23	1.65	0.61
3:X:11:LYS:HG2	3:X:12:THR:N	2.16	0.61
3:X:45:PHE:HB2	3:X:50:LEU:HD11	1.80	0.61
2:C:943:MET:HE3	2:C:947:ASN:OD1	2.00	0.61
1:B:55:HIS:HB3	1:B:66:LYS:HD2	1.82	0.61
1:A:102:VAL:O	1:A:106:ILE:HG13	2.01	0.61
2:D:869:LEU:HD13	2:D:938:ARG:NH1	2.16	0.61
3:X:5:VAL:HG21	3:X:30:ILE:HD11	1.82	0.61
2:D:815:LEU:HD23	2:D:820:ILE:HD13	1.83	0.60
2:D:713:ARG:NH1	2:D:825:GLU:HG3	2.16	0.60
2:D:783:ASN:HD22	2:D:783:ASN:C	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:TYR:CD1	1:A:61:PRO:HA	2.36	0.60
1:A:13:LEU:CD2	1:A:18:PRO:HD3	2.31	0.60
1:B:11:ASN:N	1:B:11:ASN:HD22	2.00	0.60
2:C:874:LYS:HD2	2:C:874:LYS:N	2.15	0.60
3:X:60:ASN:O	3:X:62:GLN:HG3	2.02	0.60
2:C:794:TRP:HA	2:C:798:ASN:ND2	2.17	0.59
1:A:51:PHE:CD2	2:D:868:LEU:HD11	2.34	0.59
1:A:96:ALA:HA	2:C:751:LEU:HD21	1.84	0.59
2:C:645:ARG:NH1	2:C:705:LYS:HE2	2.18	0.59
2:D:863:PHE:HA	2:D:937:LEU:HD21	1.83	0.59
1:B:56:PHE:CE2	1:B:99:ILE:HD11	2.38	0.59
2:D:779:VAL:HG23	2:D:779:VAL:O	2.03	0.59
2:C:600:MET:O	2:C:630:ILE:HA	2.03	0.59
2:C:820:ILE:HD11	2:C:828:LEU:CD1	2.33	0.59
2:D:928:LEU:HD12	2:D:929:PRO:HD2	1.85	0.58
3:Y:1:MET:HB3	3:Y:17:VAL:O	2.03	0.58
2:D:891:ASN:HD22	2:D:895:GLU:HG3	1.68	0.58
3:X:23:ILE:HA	3:X:26:VAL:HG23	1.84	0.58
2:D:604:ARG:HH11	2:D:604:ARG:HG2	1.67	0.58
2:D:844:ARG:HA	2:D:864:TRP:CZ2	2.39	0.58
3:X:22:THR:HA	3:X:54:ARG:O	2.04	0.58
2:D:686:HIS:CD2	2:D:687:LEU:H	2.21	0.58
2:D:726:LEU:HA	2:D:792:ILE:CD1	2.34	0.58
2:D:755:PHE:CD1	2:D:771:LYS:HD2	2.39	0.58
1:B:13:LEU:HD23	1:B:18:PRO:HD2	1.85	0.58
2:C:665:TYR:CD1	2:C:671:TYR:HA	2.38	0.57
2:D:815:LEU:HD23	2:D:820:ILE:CD1	2.33	0.57
1:B:98:LYS:HG3	1:B:101:LYS:CE	2.33	0.57
2:C:844:ARG:HA	2:C:864:TRP:CH2	2.39	0.57
1:A:142:THR:O	1:A:147:MET:HG3	2.04	0.57
2:C:630:ILE:HB	2:C:643:VAL:HG23	1.85	0.57
2:D:646:GLU:HG3	2:D:650:LEU:HD11	1.84	0.57
2:D:655:MET:HB3	2:D:693:ILE:HD12	1.86	0.57
1:B:55:HIS:HB3	1:B:66:LYS:CG	2.35	0.57
2:D:650:LEU:HD12	2:D:650:LEU:N	2.20	0.57
3:X:5:VAL:HG11	3:X:30:ILE:HD13	1.85	0.57
3:X:16:GLU:O	3:X:29:LYS:NZ	2.37	0.57
3:X:31:GLN:HE21	3:X:38:PRO:HD3	1.67	0.57
2:C:943:MET:HE2	2:C:947:ASN:OD1	2.04	0.56
3:Y:13:ILE:HD11	3:Y:30:ILE:HG23	1.85	0.56
2:D:757:ILE:HD11	4:D:8:HOH:O	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:HA	1:A:92:GLN:HB2	1.87	0.56
1:A:121:PRO:HG2	1:A:122:GLU:H	1.70	0.56
2:C:830:LEU:HD23	2:C:830:LEU:O	2.04	0.56
2:D:713:ARG:HD3	4:D:13:HOH:O	2.05	0.56
2:D:917:PRO:O	3:Y:73:LEU:HD22	2.05	0.56
1:B:13:LEU:HD23	1:B:18:PRO:CD	2.36	0.56
2:C:604:ARG:HH22	2:C:635:GLU:HB2	1.71	0.56
2:D:676:ASN:HD22	2:D:677:PRO:HD2	1.71	0.56
2:D:665:TYR:CD1	2:D:671:TYR:HA	2.40	0.56
2:C:607:ILE:HG23	2:C:608:PHE:N	2.20	0.56
2:D:742:TRP:O	2:D:746:ASN:ND2	2.39	0.56
2:C:856:ASN:N	2:C:856:ASN:HD22	2.03	0.56
2:C:575:PHE:O	2:C:579:GLN:HG3	2.06	0.55
1:A:26:VAL:HG21	1:A:34:GLN:OE1	2.05	0.55
1:A:130:ASP:O	1:A:133:LYS:HB3	2.06	0.55
1:A:26:VAL:HG21	1:A:34:GLN:CD	2.26	0.55
2:D:612:TYR:CE1	2:D:616:MET:HG3	2.41	0.55
2:C:849:TYR:CE1	2:C:907:ILE:HD12	2.39	0.55
2:D:869:LEU:CD1	2:D:938:ARG:NH1	2.69	0.55
1:A:7:HIS:O	1:A:10:LEU:HB3	2.07	0.55
2:C:656:PHE:HB3	2:C:673:LEU:CD1	2.37	0.55
2:D:909:GLN:HG3	2:D:930:PRO:HG3	1.88	0.55
1:A:5:ARG:NH2	1:A:61:PRO:HG3	2.21	0.55
1:B:54:ILE:HG12	1:B:67:VAL:HG22	1.88	0.55
2:D:813:GLU:HB3	2:D:814:LEU:CD1	2.37	0.55
1:A:75:HIS:ND1	1:A:76:PRO:HD2	2.22	0.55
3:X:1:MET:HB3	3:X:17:VAL:O	2.07	0.55
1:A:60:TYR:CG	1:A:61:PRO:HA	2.43	0.54
2:C:638:LEU:HA	2:C:640:TYR:CE2	2.42	0.54
2:D:783:ASN:C	2:D:783:ASN:ND2	2.61	0.54
2:C:762:PHE:O	2:C:764:GLN:NE2	2.39	0.54
1:A:50:PHE:CE1	1:A:73:ILE:HG13	2.43	0.54
1:B:2:ALA:O	1:B:3:SER:C	2.45	0.54
2:C:761:ASN:O	2:C:761:ASN:ND2	2.40	0.54
3:Y:17:VAL:HG21	3:Y:56:LEU:CD1	2.38	0.54
1:A:76:PRO:HG3	1:A:123:ILE:HG22	1.90	0.54
1:B:8:LYS:HD3	2:D:752:ASP:OD2	2.08	0.54
2:C:691:THR:HG23	2:C:806:ALA:HB1	1.90	0.54
1:B:76:PRO:HG3	1:B:123:ILE:HG22	1.90	0.53
2:D:689:TYR:O	2:D:692:PHE:HB3	2.08	0.53
2:C:697:ALA:HA	2:C:707:LEU:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:711:PHE:N	2:C:711:PHE:CD2	2.76	0.53
2:C:653:LYS:HD2	2:C:890:MET:HG3	1.89	0.53
3:X:4:PHE:HE1	3:X:14:THR:CG2	2.21	0.53
3:Y:2:GLN:HB2	3:Y:16:GLU:OE2	2.08	0.53
3:Y:61:ILE:HG21	3:Y:67:LEU:HD11	1.91	0.53
2:D:896:LEU:HD23	2:D:897:TYR:H	1.72	0.53
1:B:113:PRO:O	1:B:115:PRO:HD3	2.09	0.53
2:C:637:GLY:O	2:C:640:TYR:CE2	2.60	0.53
2:C:947:ASN:ND2	3:X:9:THR:OG1	2.41	0.53
2:D:695:ARG:HD2	2:D:813:GLU:HG2	1.90	0.53
1:B:15:ARG:HD3	1:B:16:ASP:HB2	1.90	0.53
1:B:55:HIS:HB3	1:B:66:LYS:CD	2.39	0.53
2:C:863:PHE:O	2:C:866:ALA:HB3	2.09	0.53
2:C:812:THR:CG2	2:C:817:ILE:HB	2.39	0.53
2:C:906:THR:CB	2:C:925:ARG:HG3	2.30	0.53
1:B:33:TRP:HB2	1:B:54:ILE:HB	1.91	0.52
1:A:59:ASP:HB3	1:A:63:LYS:CG	2.40	0.52
1:A:18:PRO:HB2	1:A:21:CYS:SG	2.50	0.52
1:B:131:ARG:HG3	1:B:135:ASN:ND2	2.21	0.52
1:A:36:THR:HG22	1:A:51:PHE:HD2	1.74	0.52
2:C:844:ARG:HA	2:C:864:TRP:CZ2	2.44	0.52
1:A:11:ASN:O	1:A:15:ARG:HG3	2.09	0.52
1:B:9:GLU:OE1	1:B:99:ILE:N	2.39	0.52
3:X:9:THR:HG22	3:X:9:THR:O	2.09	0.52
1:B:118:PRO:HG3	2:D:910:TRP:NE1	2.25	0.52
2:C:913:PRO:HG3	2:C:930:PRO:O	2.09	0.52
1:A:13:LEU:HD22	1:A:18:PRO:CD	2.38	0.52
1:A:25:PRO:HA	1:A:33:TRP:HA	1.91	0.52
2:C:761:ASN:N	2:C:761:ASN:HD22	2.08	0.52
3:X:26:VAL:O	3:X:30:ILE:HG13	2.10	0.52
3:Y:13:ILE:HG21	3:Y:34:GLU:OE2	2.09	0.52
1:A:39:GLY:HA3	1:A:45:TYR:O	2.10	0.52
2:C:757:ILE:HD13	2:C:794:TRP:CZ3	2.43	0.52
2:C:815:LEU:N	2:C:815:LEU:HD12	2.25	0.52
3:X:54:ARG:HG2	3:X:54:ARG:HH11	1.75	0.52
1:A:74:TYR:HB2	1:A:141:TRP:CD2	2.45	0.52
2:C:812:THR:HG21	2:C:817:ILE:HB	1.90	0.52
1:B:9:GLU:OE1	1:B:99:ILE:HG12	2.10	0.51
2:C:729:MET:CE	2:C:740:LEU:HD12	2.36	0.51
2:C:863:PHE:O	2:C:867:VAL:HG23	2.10	0.51
2:D:604:ARG:HH11	2:D:604:ARG:HG3	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:671:TYR:HE1	2:D:885:THR:HG21	1.73	0.51
3:X:67:LEU:HD12	3:X:67:LEU:H	1.75	0.51
2:D:596:ASN:O	2:D:597:ARG:HG2	2.10	0.51
2:D:638:LEU:HD23	2:D:638:LEU:N	2.24	0.51
3:X:43:LEU:HA	3:X:68:HIS:O	2.10	0.51
1:B:142:THR:O	1:B:147:MET:HG3	2.09	0.51
2:C:590:LYS:HD2	2:C:625:LYS:O	2.10	0.51
2:C:765:THR:HG23	2:C:765:THR:O	2.10	0.51
3:Y:23:ILE:CD1	3:Y:50:LEU:HD13	2.41	0.51
2:C:706:LEU:HD13	2:C:834:GLY:HA3	1.92	0.51
2:D:845:GLN:HG2	2:D:845:GLN:O	2.10	0.51
1:B:11:ASN:N	1:B:11:ASN:ND2	2.56	0.51
2:C:812:THR:HA	2:C:815:LEU:O	2.10	0.51
3:X:63:LYS:O	3:X:64:GLU:HB2	2.09	0.51
1:B:101:LYS:O	1:B:105:SER:HB2	2.11	0.51
2:D:764:GLN:HG3	2:D:766:TYR:CE1	2.46	0.51
3:X:54:ARG:HG2	3:X:54:ARG:NH1	2.26	0.51
1:A:75:HIS:ND1	1:A:76:PRO:N	2.59	0.51
1:B:75:HIS:ND1	1:B:76:PRO:CD	2.73	0.51
3:X:50:LEU:HD13	3:X:61:ILE:HD11	1.93	0.51
2:C:583:TYR:CZ	2:C:587:LYS:HD2	2.46	0.51
2:D:729:MET:O	2:D:729:MET:HG2	2.11	0.51
1:B:60:TYR:CD1	1:B:61:PRO:HA	2.45	0.50
2:C:910:TRP:HB3	2:C:927:ASP:HB3	1.92	0.50
1:A:2:ALA:CB	2:C:758:ASP:OD2	2.59	0.50
1:B:144:LYS:HB2	1:B:144:LYS:NZ	2.27	0.50
2:C:671:TYR:CZ	2:C:889:PRO:HG3	2.45	0.50
2:C:929:PRO:HG2	2:C:931:TYR:CZ	2.46	0.50
2:C:822:ILE:HG12	2:C:822:ILE:O	2.09	0.50
2:D:649:PHE:CZ	2:D:653:LYS:HE3	2.47	0.50
2:D:814:LEU:C	2:D:815:LEU:HD12	2.32	0.50
2:C:578:LYS:O	2:C:582:ASP:OD1	2.29	0.50
2:D:840:VAL:CG2	2:D:875:ARG:HD3	2.42	0.50
3:X:23:ILE:HB	3:X:51:GLU:O	2.12	0.50
1:B:36:THR:HG22	1:B:51:PHE:HD2	1.77	0.49
2:C:648:PHE:CE2	2:C:705:LYS:HG3	2.47	0.49
2:D:609:GLU:HB3	2:D:613:ARG:HH12	1.77	0.49
2:D:671:TYR:CE1	2:D:885:THR:HG21	2.47	0.49
2:D:914:GLU:HA	2:D:914:GLU:OE2	2.12	0.49
2:D:854:CYS:HB2	2:D:855:PRO:HD2	1.95	0.49
1:B:98:LYS:H	1:B:101:LYS:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ASP:OD1	1:B:117:ASP:N	2.41	0.49
2:C:604:ARG:NH1	2:C:604:ARG:HB2	2.28	0.49
2:C:910:TRP:CZ3	2:C:918:ARG:HD2	2.48	0.49
2:D:757:ILE:HD13	2:D:758:ASP:N	2.27	0.49
1:A:36:THR:CG2	2:D:868:LEU:CD1	2.90	0.49
2:C:621:PRO:O	2:C:624:LEU:HD12	2.13	0.49
3:Y:23:ILE:HB	3:Y:51:GLU:O	2.12	0.49
1:A:74:TYR:HB2	1:A:141:TRP:CE3	2.48	0.49
2:C:691:THR:HG22	2:C:806:ALA:O	2.12	0.49
2:D:643:VAL:HG23	2:D:646:GLU:H	1.78	0.49
1:A:75:HIS:ND1	1:A:76:PRO:CD	2.76	0.49
2:C:604:ARG:NH2	2:C:635:GLU:HG3	2.27	0.49
3:Y:23:ILE:HD12	3:Y:50:LEU:HD13	1.95	0.49
2:D:582:ASP:O	2:D:586:LYS:HG3	2.13	0.48
2:D:604:ARG:CG	2:D:604:ARG:NH1	2.66	0.48
2:D:794:TRP:HA	2:D:798:ASN:HD22	1.75	0.48
2:D:938:ARG:O	2:D:938:ARG:HG2	2.13	0.48
2:C:947:ASN:O	3:X:71:LEU:HD12	2.13	0.48
2:D:746:ASN:ND2	2:D:746:ASN:N	2.61	0.48
2:D:618:VAL:HA	2:D:619:LYS:HE3	1.95	0.48
1:A:19:ALA:HB1	1:A:20:GLN:HE21	1.79	0.48
2:C:705:LYS:O	2:C:706:LEU:HD23	2.13	0.48
1:A:58:THR:HG21	2:C:760:GLU:CG	2.41	0.48
2:C:794:TRP:CD1	2:C:799:ARG:HD2	2.49	0.48
2:D:869:LEU:CB	2:D:938:ARG:HH12	2.26	0.48
2:C:581:TYR:CZ	2:C:585:ARG:HD3	2.49	0.48
1:A:131:ARG:HG3	1:A:135:ASN:HD21	1.78	0.48
1:B:127:TYR:HD1	1:B:134:TYR:CG	2.32	0.48
2:C:653:LYS:CD	2:C:890:MET:HG3	2.43	0.48
2:D:650:LEU:HD12	2:D:650:LEU:H	1.78	0.48
2:D:771:LYS:HE3	2:D:786:GLU:OE2	2.13	0.48
1:B:44:PRO:HB2	1:B:138:ALA:HB3	1.95	0.47
2:D:813:GLU:C	2:D:814:LEU:HD12	2.33	0.47
1:A:36:THR:HG21	2:D:868:LEU:CD1	2.45	0.47
1:B:126:ILE:HG23	1:B:133:LYS:HG2	1.96	0.47
3:Y:13:ILE:O	3:Y:13:ILE:HG13	2.14	0.47
2:D:630:ILE:N	2:D:630:ILE:HD12	2.28	0.47
1:A:131:ARG:HG3	1:A:135:ASN:ND2	2.29	0.47
2:C:910:TRP:CZ2	2:C:918:ARG:HD2	2.47	0.47
2:D:689:TYR:O	2:D:693:ILE:HG12	2.15	0.47
1:B:75:HIS:CE1	1:B:76:PRO:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:784:LYS:O	2:C:788:ILE:HG13	2.13	0.47
2:C:702:PHE:C	2:C:702:PHE:CD2	2.87	0.47
2:D:935:GLU:O	2:D:939:GLU:HB2	2.14	0.47
1:B:5:ARG:HD3	2:D:751:LEU:O	2.15	0.47
2:C:620:ARG:O	2:C:622:ASP:N	2.48	0.47
2:C:696:VAL:O	2:C:699:LEU:HB3	2.14	0.47
1:A:59:ASP:HB3	1:A:63:LYS:HG2	1.97	0.47
1:A:64:PRO:HB3	1:A:93:TRP:CG	2.50	0.47
1:B:13:LEU:CD2	1:B:18:PRO:HD2	2.44	0.47
2:C:814:LEU:CB	2:C:815:LEU:HD12	2.45	0.47
2:D:869:LEU:HB3	2:D:938:ARG:HH12	1.80	0.47
3:Y:15:LEU:HD11	3:Y:30:ILE:HG12	1.96	0.47
1:A:147:MET:CE	2:D:856:ASN:HB3	2.45	0.46
1:A:116:ASP:C	1:A:118:PRO:HD3	2.35	0.46
2:C:608:PHE:HE2	2:C:689:TYR:CE2	2.33	0.46
3:Y:50:LEU:HD22	3:Y:59:TYR:CD2	2.51	0.46
1:B:13:LEU:CD2	1:B:18:PRO:CD	2.93	0.46
2:C:607:ILE:CD1	2:C:650:LEU:HB3	2.46	0.46
1:A:19:ALA:O	1:A:20:GLN:HB2	2.15	0.46
2:C:726:LEU:HA	2:C:792:ILE:HD13	1.97	0.46
2:C:846:HIS:HA	2:D:638:LEU:HD12	1.98	0.46
2:D:946:GLU:O	2:D:947:ASN:OD1	2.34	0.46
2:C:759:GLU:HB2	2:C:766:TYR:CE1	2.51	0.46
2:C:862:TRP:O	2:C:863:PHE:C	2.54	0.46
2:C:872:ALA:O	2:C:876:ILE:HG13	2.15	0.46
2:D:706:LEU:HD22	2:D:834:GLY:CA	2.46	0.46
2:D:909:GLN:CG	2:D:930:PRO:HG3	2.46	0.46
3:X:42:ARG:NH1	3:X:72:ARG:HE	2.14	0.46
1:A:13:LEU:HD23	1:A:18:PRO:HD3	1.96	0.46
2:D:704:GLY:C	2:D:705:LYS:HE2	2.35	0.46
1:A:99:ILE:O	1:A:100:SER:C	2.54	0.46
1:B:56:PHE:HE2	1:B:99:ILE:HD11	1.79	0.46
1:B:135:ASN:O	1:B:139:ARG:HG3	2.16	0.46
2:C:658:PRO:HG2	2:C:665:TYR:CE2	2.51	0.46
2:C:949:GLN:O	2:C:949:GLN:HG2	2.16	0.46
3:X:67:LEU:HD12	3:X:67:LEU:N	2.30	0.46
1:A:8:LYS:HE2	2:C:752:ASP:HB2	1.98	0.46
1:A:25:PRO:HB3	1:A:33:TRP:CD1	2.51	0.45
1:A:36:THR:HG22	1:A:51:PHE:CD2	2.51	0.45
2:C:906:THR:HB	2:C:925:ARG:CG	2.32	0.45
2:D:844:ARG:HG3	2:D:864:TRP:NE1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:891:ASN:HB2	2:D:895:GLU:HG3	1.97	0.45
2:C:599:GLU:O	2:C:614:ARG:NH1	2.49	0.45
2:D:597:ARG:CB	2:D:597:ARG:HH11	2.28	0.45
2:D:691:THR:O	2:D:691:THR:CG2	2.64	0.45
1:A:60:TYR:CE2	1:A:61:PRO:HB3	2.50	0.45
2:D:691:THR:O	2:D:691:THR:HG22	2.16	0.45
3:X:37:PRO:HA	3:X:38:PRO:HD3	1.87	0.45
1:A:29:ASP:OD1	1:A:31:PHE:N	2.41	0.45
2:D:757:ILE:HD13	2:D:758:ASP:H	1.81	0.45
2:D:912:SER:O	2:D:914:GLU:N	2.50	0.45
3:X:21:ASP:O	3:X:55:THR:HA	2.15	0.45
2:C:699:LEU:HD12	2:C:703:HIS:CD2	2.51	0.45
2:C:919:ALA:O	3:X:74:ARG:HG3	2.16	0.45
1:B:126:ILE:CG2	1:B:133:LYS:HG2	2.47	0.45
2:C:873:GLU:OE2	2:C:874:LYS:NZ	2.50	0.45
1:A:72:ARG:HB2	1:A:145:TYR:CG	2.51	0.45
2:C:665:TYR:CE1	2:C:671:TYR:HA	2.52	0.45
2:C:702:PHE:C	2:C:702:PHE:HD2	2.20	0.45
2:D:588:LEU:HD23	2:D:819:LEU:HD23	1.99	0.45
2:D:773:ASN:HD21	2:D:776:GLU:HG3	1.82	0.45
3:Y:59:TYR:O	3:Y:60:ASN:HB2	2.17	0.45
1:B:69:PHE:O	1:B:82:GLY:HA3	2.17	0.45
2:C:729:MET:HB2	2:C:796:PHE:HE2	1.81	0.45
2:D:686:HIS:CD2	2:D:687:LEU:N	2.83	0.45
2:D:910:TRP:O	2:D:929:PRO:HA	2.16	0.45
2:C:856:ASN:N	2:C:856:ASN:ND2	2.65	0.44
2:C:910:TRP:O	2:C:929:PRO:HA	2.17	0.44
2:D:864:TRP:HA	2:D:864:TRP:CE3	2.52	0.44
1:A:45:TYR:HE1	1:A:110:LEU:O	2.01	0.44
1:B:37:ILE:HD12	1:B:52:LEU:HD11	1.99	0.44
1:B:128:LYS:HD3	1:B:128:LYS:HA	1.42	0.44
2:C:657:ASN:ND2	2:C:890:MET:CE	2.80	0.44
2:C:769:ASP:OD1	2:C:775:SER:HB3	2.17	0.44
2:C:865:LYS:O	2:C:869:LEU:HG	2.17	0.44
2:D:604:ARG:HG3	2:D:604:ARG:NH1	2.30	0.44
1:A:13:LEU:O	1:A:17:PRO:CG	2.64	0.44
2:C:743:ILE:O	2:C:784:LYS:HD2	2.18	0.44
2:C:828:LEU:HD12	2:C:828:LEU:O	2.17	0.44
2:D:602:LEU:HD12	2:D:602:LEU:O	2.17	0.44
1:A:63:LYS:HD3	2:C:736:TYR:HD2	1.82	0.44
2:C:648:PHE:CE1	2:C:700:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:699:LEU:HD12	2:C:703:HIS:HD2	1.83	0.44
3:X:42:ARG:HG3	3:X:72:ARG:CG	2.45	0.44
2:C:662:LEU:HD23	2:C:662:LEU:HA	1.81	0.44
2:D:854:CYS:HB2	2:D:855:PRO:CD	2.47	0.44
2:D:931:TYR:CE1	2:D:940:LYS:HG2	2.53	0.44
1:A:22:SER:OG	1:A:36:THR:OG1	2.36	0.44
1:A:62:PHE:HD1	2:C:736:TYR:CZ	2.35	0.44
2:C:740:LEU:HD23	2:C:740:LEU:HA	1.82	0.44
2:C:759:GLU:HB2	2:C:766:TYR:CZ	2.53	0.44
2:D:754:MET:HA	2:D:777:ILE:O	2.18	0.44
2:D:876:ILE:HG22	2:D:886:SER:HB2	1.99	0.44
3:Y:9:THR:O	3:Y:11:LYS:N	2.50	0.44
2:D:591:PRO:HG2	2:D:594:ILE:HG21	1.99	0.43
3:Y:45:PHE:HB3	3:Y:50:LEU:HD21	1.99	0.43
2:C:652:SER:C	2:C:654:GLU:N	2.72	0.43
2:C:710:PHE:CE1	2:C:833:CYS:O	2.71	0.43
2:C:729:MET:HG3	2:C:796:PHE:HZ	1.82	0.43
2:D:889:PRO:HG2	2:D:892:GLY:O	2.18	0.43
2:C:895:GLU:OE1	2:D:631:GLU:OE2	2.37	0.43
2:D:912:SER:C	2:D:914:GLU:H	2.21	0.43
1:A:60:TYR:CZ	1:A:61:PRO:HB3	2.54	0.43
2:C:652:SER:O	2:C:654:GLU:N	2.51	0.43
2:C:795:ARG:CG	2:C:795:ARG:HH11	2.32	0.43
2:D:876:ILE:CG2	2:D:886:SER:HB2	2.49	0.43
3:Y:9:THR:C	3:Y:11:LYS:N	2.71	0.43
2:C:618:VAL:HG21	2:C:624:LEU:HD11	2.01	0.43
3:Y:22:THR:HA	3:Y:55:THR:HA	2.00	0.43
2:D:949:GLN:OE1	2:D:949:GLN:N	2.40	0.43
3:Y:23:ILE:HG13	3:Y:50:LEU:HB3	2.01	0.43
3:X:11:LYS:CG	3:X:12:THR:N	2.81	0.43
1:A:59:ASP:HB3	1:A:63:LYS:HG3	2.01	0.42
2:C:611:SER:O	2:C:615:ILE:HG12	2.19	0.42
2:C:630:ILE:HB	2:C:643:VAL:CG2	2.49	0.42
2:C:633:GLU:HA	2:C:636:LYS:HE3	2.01	0.42
2:C:648:PHE:HE2	2:C:705:LYS:HG3	1.83	0.42
2:C:891:ASN:HB2	2:C:895:GLU:HG3	2.02	0.42
2:D:699:LEU:HD13	2:D:814:LEU:HD21	2.00	0.42
2:D:880:GLN:HA	2:D:885:THR:O	2.19	0.42
2:C:850:LYS:NZ	2:C:906:THR:HG21	2.34	0.42
2:D:773:ASN:ND2	2:D:776:GLU:HG3	2.35	0.42
2:D:850:LYS:O	2:D:908:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:HH11	1:A:72:ARG:CG	2.30	0.42
1:A:75:HIS:CE1	1:A:76:PRO:HD2	2.54	0.42
1:B:2:ALA:HA	1:B:6:ILE:HG13	2.01	0.42
2:C:712:ILE:HA	4:C:3:HOH:O	2.19	0.42
2:D:840:VAL:O	2:D:840:VAL:HG12	2.19	0.42
2:D:912:SER:C	2:D:914:GLU:N	2.73	0.42
3:X:4:PHE:CE2	3:X:64:GLU:HG3	2.54	0.42
2:D:646:GLU:O	2:D:650:LEU:HD13	2.20	0.42
3:X:15:LEU:HD11	3:X:30:ILE:HG12	2.01	0.42
1:A:7:HIS:O	1:A:10:LEU:N	2.53	0.42
2:C:608:PHE:CE1	2:C:655:MET:HG2	2.54	0.42
2:C:822:ILE:O	2:C:822:ILE:CG1	2.68	0.42
2:C:824:ASP:H	2:C:827:GLU:HB2	1.84	0.42
2:C:918:ARG:HH12	3:X:75:GLY:HA2	1.84	0.42
2:C:632:PHE:CE1	2:C:646:GLU:OE1	2.72	0.42
3:X:6:LYS:HB3	3:X:68:HIS:CD2	2.54	0.42
1:A:136:ARG:HG2	1:A:136:ARG:HH11	1.84	0.42
2:D:942:LEU:HD23	2:D:942:LEU:HA	1.93	0.42
1:B:116:ASP:O	1:B:118:PRO:HD2	2.14	0.42
2:D:713:ARG:HB3	2:D:714:PRO:CD	2.43	0.42
2:D:823:PHE:HB3	2:D:827:GLU:HB2	2.00	0.42
3:Y:72:ARG:HA	3:Y:72:ARG:HD3	1.40	0.42
1:A:16:ASP:N	1:A:17:PRO:HD3	2.35	0.41
2:C:848:ILE:CG1	2:C:906:THR:HG23	2.39	0.41
2:D:880:GLN:C	2:D:882:VAL:N	2.72	0.41
2:C:770:LEU:HD23	2:C:770:LEU:HA	1.91	0.41
2:C:839:ASP:OD1	2:C:839:ASP:C	2.58	0.41
3:Y:13:ILE:CD1	3:Y:30:ILE:HG23	2.49	0.41
3:Y:28:ALA:O	3:Y:32:ASP:OD1	2.38	0.41
2:C:671:TYR:CE1	2:C:889:PRO:HD3	2.56	0.41
1:B:50:PHE:CE1	1:B:146:ALA:HB2	2.56	0.41
2:D:838:VAL:HG11	2:D:843:TRP:CE3	2.55	0.41
2:C:612:TYR:O	2:C:616:MET:HB2	2.21	0.41
2:C:851:ASN:ND2	2:C:909:GLN:O	2.51	0.41
3:Y:42:ARG:NH2	3:Y:49:GLN:OE1	2.50	0.41
1:B:130:ASP:OD2	1:B:133:LYS:HB2	2.20	0.41
1:A:13:LEU:CD2	1:A:18:PRO:CD	2.96	0.41
2:D:594:ILE:HD12	2:D:626:ALA:HB2	2.03	0.41
2:D:844:ARG:HG3	2:D:864:TRP:CE2	2.56	0.41
3:Y:9:THR:C	3:Y:11:LYS:H	2.23	0.41
2:C:794:TRP:CA	2:C:798:ASN:HD22	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:871:ASP:O	2:C:872:ALA:C	2.59	0.41
2:D:712:ILE:HB	2:D:732:VAL:HG22	2.03	0.41
2:C:762:PHE:CD1	2:C:762:PHE:N	2.86	0.41
2:C:802:LYS:HB3	2:C:802:LYS:NZ	2.36	0.41
2:C:818:ASP:HA	2:C:821:LYS:HG3	2.02	0.41
2:D:676:ASN:HD22	2:D:677:PRO:CD	2.33	0.41
2:D:781:ASN:HD22	2:D:781:ASN:C	2.23	0.41
3:Y:4:PHE:HB3	3:Y:12:THR:HG21	2.02	0.41
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.85	0.41
2:C:794:TRP:CA	2:C:798:ASN:ND2	2.82	0.41
2:C:938:ARG:HG2	2:C:942:LEU:HD12	2.02	0.41
2:D:635:GLU:H	2:D:635:GLU:HG3	1.45	0.41
2:D:668:THR:HG22	2:D:897:TYR:CD2	2.56	0.41
2:D:893:PHE:CD1	2:D:896:LEU:HD12	2.56	0.41
2:D:928:LEU:HD12	2:D:929:PRO:CD	2.50	0.41
2:C:585:ARG:O	2:C:588:LEU:HB2	2.22	0.40
2:D:577:PHE:CZ	2:D:830:LEU:HD23	2.55	0.40
2:D:835:LEU:HD23	2:D:835:LEU:HA	1.88	0.40
1:A:121:PRO:HG2	1:A:122:GLU:N	2.35	0.40
1:B:131:ARG:CG	1:B:135:ASN:HD21	2.25	0.40
2:C:609:GLU:O	2:C:612:TYR:HB3	2.21	0.40
2:D:713:ARG:NH1	2:D:717:LYS:HD2	2.36	0.40
3:X:31:GLN:HE21	3:X:37:PRO:HA	1.86	0.40
2:D:896:LEU:HD22	2:D:924:ASN:ND2	2.36	0.40
1:B:92:GLN:NE2	1:B:92:GLN:HA	2.36	0.40
2:C:591:PRO:HG2	2:C:594:ILE:HD13	2.04	0.40
2:C:659:TYR:HE2	2:D:627:ARG:HH21	1.68	0.40
2:D:733:ASP:OD2	2:D:736:TYR:CB	2.54	0.40
1:A:18:PRO:HG2	1:A:21:CYS:SG	2.61	0.40
1:B:35:ALA:O	1:B:51:PHE:HA	2.21	0.40
1:B:79:ASN:ND2	1:B:83:SER:HB2	2.37	0.40
2:D:622:ASP:C	2:D:624:LEU:H	2.25	0.40
2:D:814:LEU:N	2:D:814:LEU:CD1	2.82	0.40
2:D:906:THR:HB	2:D:925:ARG:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/146 (99%)	130 (90%)	14 (10%)	0	100	100
1	B	144/146 (99%)	132 (92%)	11 (8%)	1 (1%)	22	57
2	C	374/385 (97%)	310 (83%)	61 (16%)	3 (1%)	19	54
2	D	372/385 (97%)	315 (85%)	56 (15%)	1 (0%)	41	73
3	X	74/81 (91%)	66 (89%)	8 (11%)	0	100	100
3	Y	74/81 (91%)	65 (88%)	9 (12%)	0	100	100
All	All	1182/1224 (97%)	1018 (86%)	159 (14%)	5 (0%)	34	69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	686	HIS
2	D	881	PHE
2	C	595	PRO
2	C	800	VAL
1	B	44	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/130 (100%)	123 (95%)	7 (5%)	22	53
1	B	130/130 (100%)	117 (90%)	13 (10%)	7	28
2	C	341/348 (98%)	315 (92%)	26 (8%)	13	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	340/348 (98%)	305 (90%)	35 (10%)	7	27
3	X	68/70 (97%)	64 (94%)	4 (6%)	19	50
3	Y	68/70 (97%)	63 (93%)	5 (7%)	13	42
All	All	1077/1096 (98%)	987 (92%)	90 (8%)	11	38

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	63	LYS
1	A	77	ASN
1	A	91	SER
1	A	100	SER
1	A	111	CYS
1	A	134	TYR
1	B	3	SER
1	B	13	LEU
1	B	15	ARG
1	B	21	CYS
1	B	66	LYS
1	B	85	SER
1	B	87	ASP
1	B	91	SER
1	B	92	GLN
1	B	105	SER
1	B	117	ASP
1	B	128	LYS
1	B	129	THR
2	C	605	ASN
2	C	614	ARG
2	C	632	PHE
2	C	634	SER
2	C	640	TYR
2	C	650	LEU
2	C	668	THR
2	C	670	ASN
2	C	686	HIS
2	C	695	ARG
2	C	702	PHE
2	C	713	ARG
2	C	718	MET

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Mol	Chain	Res	Type
2	C	727	ASN
2	C	761	ASN
2	C	768	VAL
2	C	795	ARG
2	C	822	ILE
2	C	825	GLU
2	C	835	LEU
2	C	841	ASN
2	C	868	LEU
2	C	874	LYS
2	C	896	LEU
2	C	913	PRO
2	C	943	MET
2	D	585	ARG
2	D	597	ARG
2	D	604	ARG
2	D	614	ARG
2	D	619	LYS
2	D	633	GLU
2	D	635	GLU
2	D	638	LEU
2	D	646	GLU
2	D	671	TYR
2	D	686	HIS
2	D	695	ARG
2	D	705	LYS
2	D	727	ASN
2	D	746	ASN
2	D	748	PRO
2	D	750	GLU
2	D	757	ILE
2	D	761	ASN
2	D	765	THR
2	D	767	GLN
2	D	769	ASP
2	D	771	LYS
2	D	781	ASN
2	D	783	ASN
2	D	789	ASP
2	D	802	LYS
2	D	814	LEU
2	D	820	ILE

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Mol	Chain	Res	Type
2	D	835	LEU
2	D	841	ASN
2	D	860	ILE
2	D	897	TYR
2	D	918	ARG
2	D	932	GLU
3	X	39	ASP
3	X	49	GLN
3	X	58	ASP
3	X	72	ARG
3	Y	19	PRO
3	Y	52	ASP
3	Y	58	ASP
3	Y	64	GLU
3	Y	72	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	32	HIS
1	A	55	HIS
1	A	135	ASN
1	B	7	HIS
1	B	11	ASN
1	B	32	HIS
1	B	41	ASN
1	B	55	HIS
1	B	135	ASN
1	B	143	GLN
2	C	678	ASN
2	C	703	HIS
2	C	723	GLN
2	C	761	ASN
2	C	793	GLN
2	C	798	ASN
2	C	856	ASN
2	C	861	GLN
2	C	891	ASN
2	D	596	ASN
2	D	676	ASN
2	D	727	ASN

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Mol	Chain	Res	Type
2	D	738	ASN
2	D	746	ASN
2	D	773	ASN
2	D	783	ASN
2	D	891	ASN
2	D	900	ASN
3	X	2	GLN
3	X	25	ASN
3	X	31	GLN
3	X	60	ASN
3	X	62	GLN
3	X	68	HIS
3	Y	62	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 monosaccharides 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	A	146/146 (100%)	0.24	3 (2%) 63 43	74, 102, 110, 110	0
1	B	146/146 (100%)	0.27	2 (1%) 75 56	73, 98, 110, 110	0
2	C	376/385 (97%)	0.20	2 (0%) 91 81	64, 96, 110, 110	0
2	D	374/385 (97%)	0.11	0 100 100	63, 90, 110, 110	0
3	X	76/81 (93%)	1.84	31 (40%) 0 0	107, 110, 110, 110	0
3	Y	76/81 (93%)	1.58	25 (32%) 0 0	105, 110, 110, 110	0
All	All	1194/1224 (97%)	0.38	63 (5%) 26 12	63, 98, 110, 110	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	65	SER	6.1
3	X	66	THR	5.8
3	X	23	ILE	5.2
3	X	3	ILE	4.9
3	X	2	GLN	4.8
3	X	5	VAL	4.7
3	X	1	MET	4.6
3	X	13	ILE	4.4
3	X	12	THR	4.2
3	Y	15	LEU	3.9
3	Y	1	MET	3.8
3	Y	13	ILE	3.8
3	Y	67	LEU	3.5
3	Y	34	GLU	3.5
3	X	59	TYR	3.4
3	X	63	LYS	3.3
3	X	64	GLU	3.2
3	X	22	THR	3.2
3	Y	68	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
3	X	4	PHE	3.1
1	A	30	MET	3.1
3	X	61	ILE	3.0
3	Y	35	GLY	3.0
3	X	21	ASP	3.0
3	X	50	LEU	3.0
3	X	9	THR	3.0
3	Y	2	GLN	2.9
3	Y	23	ILE	2.9
3	X	49	GLN	2.9
3	X	8	LEU	2.9
3	X	41	GLN	2.8
3	Y	21	ASP	2.8
3	Y	54	ARG	2.7
3	Y	64	GLU	2.7
3	Y	66	THR	2.7
3	X	45	PHE	2.7
3	Y	14	THR	2.7
3	X	30	ILE	2.7
3	Y	12	THR	2.7
3	Y	22	THR	2.7
3	Y	43	LEU	2.6
3	Y	17	VAL	2.6
3	Y	5	VAL	2.5
3	Y	52	ASP	2.5
3	Y	59	TYR	2.4
3	Y	36	ILE	2.4
3	X	51	GLU	2.4
1	A	18	PRO	2.3
1	B	21	CYS	2.3
3	X	44	ILE	2.3
3	Y	11	LYS	2.3
3	X	14	THR	2.3
3	X	67	LEU	2.2
1	A	130	ASP	2.2
3	Y	58	ASP	2.1
2	C	583	TYR	2.1
3	X	56	LEU	2.1
3	X	34	GLU	2.1
1	B	42	ASP	2.1
3	X	60	ASN	2.1
2	C	575	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	Y	44	ILE	2.1
3	X	54	ARG	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 monosaccharides 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.