



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 12:50 PM EDT

PDB ID : 3JVZ
Title : E2 Ubiquitin-HECT
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Deposited on : 2009-09-17
Resolution : 3.30 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 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

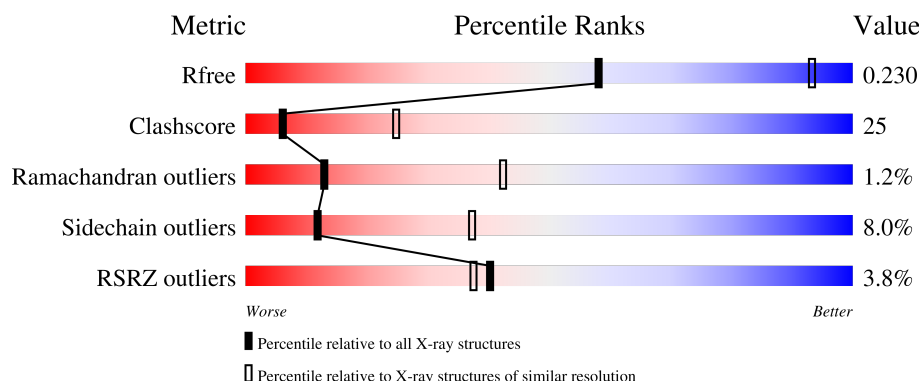
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	<div><div></div><div>25%</div><div>44%</div><div>46%</div><div>•</div><div>6%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9814 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
1	A	146	Total	C	N	O	S	0	0	0
			1170	749	202	213	6			
1	B	146	Total	C	N	O	S	0	0	0
			1170	749	202	213	6			

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
2	C	377	Total	C	N	O	S	0	0	0
			3148	2037	520	574	17			
2	D	374	Total	C	N	O	S	0	0	0
			3124	2021	517	569	17			

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	ALA	CYS	engineered mutation	UNP Q96PU5

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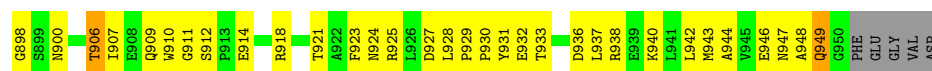
Chain	Residue	Modelled	Actual	Comment	Reference
D	571	GLY	-	expression tag	UNP Q96PU5
D	572	SER	-	expression tag	UNP Q96PU5
D	573	PRO	-	expression tag	UNP Q96PU5
D	574	GLU	-	expression tag	UNP Q96PU5
D	575	PHE	-	expression tag	UNP Q96PU5
D	922	ALA	CYS	engineered mutation	UNP Q96PU5

- Molecule 3 is a protein called Ubiquitin.

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

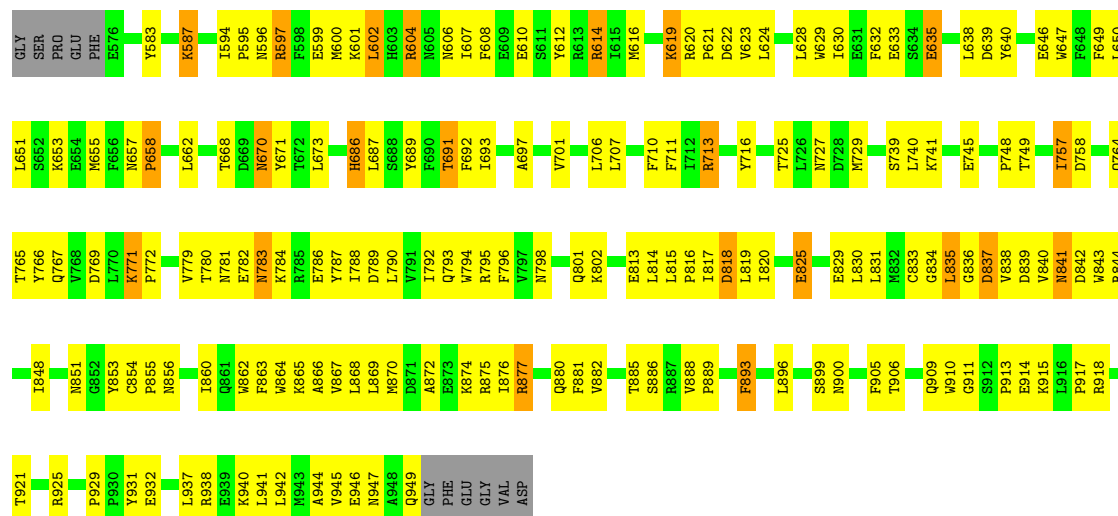
There are 10 discrepancies between the modelled and reference sequences:

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 2: E3 ubiquitin-protein ligase NEDD4-like

Chain D: 51% 41% 6%



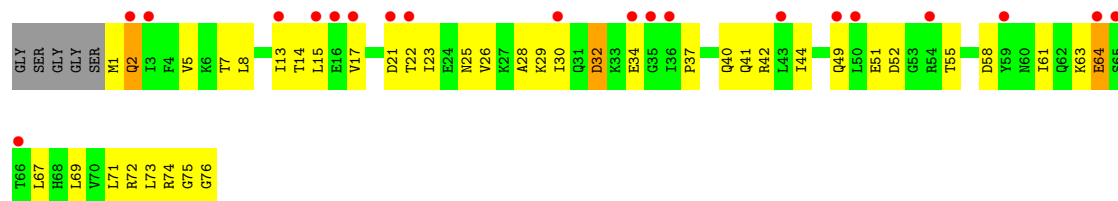
• Molecule 3: Ubiquitin

Chain X: 28% 46% 44% 6%



• Molecule 3: Ubiquitin

Chain Y: 25% 44% 46% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	173.98Å 199.89Å 109.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.97 – 3.30	Depositor EDS
% Data completeness (in resolution range)	87.5 (50.00-3.30) 87.4 (49.97-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.267 0.220 , 0.230	Depositor DCC
R_{free} test set	1288 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	74.2	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9814	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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	0.43	0/1206	0.67	0/1642
1	B	0.41	0/1206	0.63	0/1642
2	C	0.49	0/3232	0.66	0/4366
2	D	0.48	1/3207 (0.0%)	0.72	1/4333 (0.0%)
3	X	0.40	0/607	0.70	0/816
3	Y	0.38	0/607	0.58	0/816
All	All	0.46	1/10065 (0.0%)	0.67	1/13615 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	837	ASP	CB-CG	5.05	1.62	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	764	GLN	N-CA-C	-5.95	94.94	111.00

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	57	0
1	B	1170	0	1152	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3148	0	3063	163	0
2	D	3124	0	3045	150	0
3	X	601	0	629	41	0
3	Y	601	0	629	40	0
All	All	9814	0	9670	480	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 (480) 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)
2:D:597:ARG:HG3	2:D:597:ARG:HH11	1.25	1.00
2:C:817:ILE:O	2:C:820:ILE:HG22	1.61	1.00
2:C:675:ILE:HD12	2:C:675:ILE:H	1.26	0.97
2:C:848:ILE:HG13	2:C:906:THR:HG23	1.49	0.95
2:C:944:ALA:O	2:C:948:ALA:HB2	1.69	0.92
3:X:7:THR:HG22	3:X:69:LEU:HD23	1.54	0.89
3:Y:41:GLN:HB2	3:Y:69:LEU:HD11	1.56	0.86
2:C:817:ILE:O	2:C:820:ILE:CG2	2.23	0.86
3:X:1:MET:SD	3:X:19:PRO:HG3	2.17	0.84
3:X:5:VAL:HB	3:X:13:ILE:HB	1.60	0.82
2:C:618:VAL:HG11	2:C:624:LEU:HD21	1.61	0.82
1:A:51:PHE:CE2	2:D:868:LEU:HD11	2.16	0.81
2:D:779:VAL:HG23	2:D:779:VAL:O	1.83	0.79
2:C:910:TRP:CH2	2:C:918:ARG:HD2	2.17	0.79
3:Y:25:ASN:O	3:Y:29:LYS:HG2	1.81	0.79
2:D:619:LYS:CE	2:D:619:LYS:H	1.96	0.78
1:A:40:PRO:HD3	1:A:110:LEU:HD23	1.63	0.78
1:B:125:ARG:NH1	1:B:125:ARG:HB3	1.98	0.78
3:X:4:PHE:CD1	3:X:14:THR:HG22	2.18	0.78
2:D:794:TRP:HA	2:D:798:ASN:HD22	1.48	0.77
2:D:740:LEU:HD13	2:D:792:ILE:HD11	1.68	0.76
3:X:13:ILE:HG23	3:X:33:LYS:HD3	1.68	0.76
2:C:871:ASP:OD1	2:C:874:LYS:HD3	1.86	0.76
2:C:876:ILE:HG22	2:C:886:SER:HB2	1.68	0.75
3:X:45:PHE:HB3	3:X:50:LEU:HD21	1.66	0.75
2:D:599:GLU:HB2	2:D:629:TRP:CE3	2.22	0.73
2:D:837:ASP:OD1	2:D:872:ALA:HB1	1.88	0.73
2:D:597:ARG:HG3	2:D:597:ARG:NH1	2.01	0.73
3:X:13:ILE:HA	3:X:33:LYS:NZ	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:PRO:HB2	1:B:138:ALA:HB3	1.71	0.73
2:D:619:LYS:H	2:D:619:LYS:HE3	1.52	0.73
1:A:102:VAL:O	1:A:106:ILE:HG13	1.88	0.73
2:D:794:TRP:HA	2:D:798:ASN:ND2	2.03	0.73
2:C:764:GLN:HE21	2:C:764:GLN:N	1.87	0.73
1:B:125:ARG:HB3	1:B:125:ARG:HH11	1.54	0.72
3:X:13:ILE:HA	3:X:33:LYS:HZ1	1.55	0.72
2:C:876:ILE:CG2	2:C:886:SER:HB2	2.20	0.72
2:D:646:GLU:HG3	2:D:650:LEU:HD13	1.71	0.71
3:X:4:PHE:CE1	3:X:14:THR:HG22	2.26	0.71
3:X:15:LEU:HD22	3:X:29:LYS:HE3	1.73	0.71
2:D:815:LEU:HD23	2:D:820:ILE:HD13	1.74	0.70
1:A:135:ASN:HB3	1:A:139:ARG:HH12	1.57	0.70
2:D:686:HIS:CD2	2:D:687:LEU:H	2.10	0.69
2:D:780:THR:OG1	2:D:782:GLU:HG2	1.93	0.69
2:C:706:LEU:HD13	2:C:834:GLY:HA3	1.75	0.68
2:C:844:ARG:HG3	2:C:864:TRP:CE2	2.29	0.68
1:B:130:ASP:OD2	1:B:133:LYS:HB2	1.94	0.67
2:D:630:ILE:HG12	2:D:647:TRP:HB2	1.75	0.67
2:C:675:ILE:HD12	2:C:675:ILE:N	2.07	0.67
2:D:713:ARG:NH2	2:D:825:GLU:HG3	2.09	0.67
2:C:675:ILE:H	2:C:675:ILE:CD1	1.95	0.67
3:X:67:LEU:HD12	3:X:67:LEU:H	1.60	0.67
2:D:740:LEU:HD13	2:D:792:ILE:CD1	2.24	0.67
2:C:729:MET:O	2:C:729:MET:HG3	1.93	0.66
2:D:862:TRP:O	2:D:865:LYS:HB3	1.95	0.66
1:A:122:GLU:O	1:A:126:ILE:HD13	1.95	0.66
1:A:136:ARG:HG2	1:A:140:GLU:OE2	1.96	0.66
2:C:604:ARG:HH22	2:C:635:GLU:HB2	1.59	0.66
1:A:90:ARG:HG2	1:A:90:ARG:HH11	1.61	0.66
2:C:761:ASN:N	2:C:761:ASN:HD22	1.93	0.66
3:Y:1:MET:HG2	3:Y:2:GLN:H	1.59	0.66
2:C:848:ILE:CG1	2:C:906:THR:HG23	2.25	0.65
2:D:853:TYR:CD2	2:D:860:ILE:HD11	2.32	0.65
2:C:931:TYR:CE1	2:C:940:LYS:HG3	2.31	0.65
2:D:921:THR:HG23	3:Y:74:ARG:HD2	1.78	0.65
3:Y:7:THR:HG22	3:Y:69:LEU:HB3	1.78	0.65
2:D:729:MET:HE2	2:D:795:ARG:HD2	1.78	0.65
1:B:9:GLU:OE1	1:B:99:ILE:N	2.25	0.65
2:C:645:ARG:NH1	2:C:705:LYS:HE2	2.12	0.65
3:Y:63:LYS:HG3	3:Y:64:GLU:OE1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:794:TRP:HA	2:C:798:ASN:HD22	1.61	0.64
1:B:144:LYS:HD3	1:B:145:TYR:CZ	2.33	0.63
1:A:76:PRO:HG3	1:A:123:ILE:HG22	1.80	0.63
1:B:113:PRO:O	1:B:115:PRO:HD3	1.98	0.63
2:D:877:ARG:NH1	2:D:877:ARG:HB3	2.14	0.63
2:D:947:ASN:HB2	3:Y:71:LEU:HD12	1.80	0.63
1:A:15:ARG:HG2	1:A:15:ARG:HH21	1.63	0.63
2:C:615:ILE:O	2:C:618:VAL:HG22	1.98	0.63
2:C:933:THR:OG1	2:C:936:ASP:HB2	1.99	0.63
2:D:918:ARG:HD2	3:Y:40:GLN:NE2	2.14	0.63
2:D:844:ARG:HA	2:D:864:TRP:CZ2	2.34	0.62
3:X:31:GLN:O	3:X:31:GLN:HG2	1.99	0.62
1:B:14:ALA:O	1:B:17:PRO:HD3	1.99	0.62
2:C:665:TYR:CD1	2:C:671:TYR:HA	2.34	0.62
3:X:63:LYS:HE3	3:X:64:GLU:OE1	2.00	0.62
1:B:2:ALA:HB1	1:B:5:ARG:HB3	1.80	0.62
2:D:915:LYS:HA	3:Y:37:PRO:HG2	1.80	0.62
3:X:50:LEU:HD13	3:X:61:ILE:HD11	1.82	0.62
2:C:608:PHE:HE1	2:C:655:MET:HA	1.64	0.62
2:D:649:PHE:HD2	2:D:650:LEU:HD12	1.65	0.62
1:A:31:PHE:CE2	2:C:765:THR:HG21	2.36	0.61
3:X:45:PHE:CZ	3:X:65:SER:HB3	2.34	0.61
3:X:18:GLU:O	3:X:56:LEU:HD12	2.00	0.61
2:C:695:ARG:O	2:C:814:LEU:HD11	2.00	0.61
1:B:144:LYS:HD3	1:B:145:TYR:CE1	2.36	0.60
2:C:784:LYS:O	2:C:788:ILE:HG13	2.00	0.60
2:D:602:LEU:HD13	2:D:607:ILE:HG13	1.83	0.60
2:D:877:ARG:HB3	2:D:877:ARG:HH11	1.65	0.60
1:A:147:MET:CE	2:D:856:ASN:HB3	2.31	0.60
2:C:581:TYR:O	2:C:584:PHE:HB3	2.01	0.60
3:X:45:PHE:HB2	3:X:50:LEU:HD11	1.82	0.60
1:B:63:LYS:NZ	1:B:63:LYS:HB3	2.16	0.60
2:C:757:ILE:HD12	2:C:768:VAL:HG13	1.82	0.60
3:Y:22:THR:O	3:Y:26:VAL:HG23	2.02	0.60
2:D:842:ASP:OD2	2:D:893:PHE:HB2	2.02	0.59
1:B:18:PRO:HG2	1:B:21:CYS:HB2	1.84	0.59
2:C:856:ASN:N	2:C:856:ASN:HD22	2.00	0.59
2:D:687:LEU:O	2:D:691:THR:HG23	2.02	0.59
1:A:147:MET:HE2	2:D:856:ASN:HB3	1.85	0.59
1:A:135:ASN:HB3	1:A:139:ARG:NH1	2.17	0.59
2:C:910:TRP:CZ2	2:C:918:ARG:HD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:762:PHE:O	2:C:764:GLN:NE2	2.36	0.59
2:C:844:ARG:HA	2:C:864:TRP:CZ2	2.38	0.59
2:C:755:PHE:CD1	2:C:771:LYS:HE2	2.38	0.58
2:D:765:THR:HG23	2:D:765:THR:O	2.03	0.58
2:C:849:TYR:HE1	2:C:907:ILE:HD12	1.68	0.58
2:C:630:ILE:O	2:C:643:VAL:HG21	2.03	0.58
2:D:839:ASP:OD2	2:D:842:ASP:HB2	2.04	0.58
2:D:671:TYR:CZ	2:D:889:PRO:HG3	2.38	0.58
2:C:686:HIS:CD2	2:C:687:LEU:H	2.21	0.58
2:D:918:ARG:HD2	3:Y:40:GLN:HE22	1.69	0.58
2:D:851:ASN:O	2:D:909:GLN:HB3	2.03	0.57
2:D:882:VAL:HG11	2:D:905:PHE:CE1	2.38	0.57
1:A:54:ILE:HG12	1:A:67:VAL:HG22	1.85	0.57
2:C:583:TYR:CZ	2:C:587:LYS:HD2	2.39	0.57
2:D:689:TYR:O	2:D:692:PHE:HB3	2.04	0.57
2:D:813:GLU:C	2:D:814:LEU:HD12	2.25	0.57
2:C:743:ILE:O	2:C:784:LYS:HD2	2.05	0.57
2:D:599:GLU:HB2	2:D:629:TRP:HE3	1.66	0.57
2:D:840:VAL:CG2	2:D:875:ARG:HD3	2.35	0.57
1:B:115:PRO:HG2	1:B:128:LYS:HE2	1.86	0.57
2:D:779:VAL:O	2:D:779:VAL:CG2	2.52	0.57
2:C:658:PRO:HG2	2:C:665:TYR:CE2	2.39	0.57
3:Y:17:VAL:HG12	3:Y:29:LYS:NZ	2.20	0.57
1:B:13:LEU:HD23	1:B:18:PRO:HD3	1.86	0.56
2:C:938:ARG:HG2	2:C:942:LEU:HD12	1.87	0.56
2:C:947:ASN:ND2	3:X:9:THR:OG1	2.39	0.56
2:D:606:ASN:ND2	2:D:610:GLU:HG3	2.21	0.56
3:Y:61:ILE:HG21	3:Y:67:LEU:HD11	1.87	0.56
1:A:23:ALA:HB2	1:A:35:ALA:HB2	1.88	0.56
2:C:794:TRP:HA	2:C:798:ASN:ND2	2.20	0.56
2:C:870:MET:HB3	2:C:874:LYS:HB2	1.87	0.56
1:B:125:ARG:HH11	1:B:125:ARG:CB	2.16	0.56
1:A:26:VAL:HG21	1:A:34:GLN:CD	2.25	0.56
2:D:848:ILE:HG13	2:D:906:THR:HG23	1.88	0.56
3:X:43:LEU:HA	3:X:68:HIS:O	2.05	0.56
2:C:812:THR:HG22	2:C:817:ILE:HB	1.89	0.55
1:B:41:ASN:O	1:B:42:ASP:HB2	2.06	0.55
2:C:801:GLN:O	2:C:805:ASN:HB2	2.05	0.55
2:C:844:ARG:HA	2:C:864:TRP:CH2	2.41	0.55
2:D:689:TYR:O	2:D:693:ILE:HG12	2.06	0.55
1:A:75:HIS:ND1	1:A:76:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:608:PHE:CE1	2:C:655:MET:HA	2.41	0.55
2:C:855:PRO:C	2:C:856:ASN:HD22	2.10	0.55
1:B:126:ILE:HD12	1:B:133:LYS:NZ	2.22	0.55
2:D:651:LEU:O	2:D:655:MET:HG3	2.07	0.55
3:Y:15:LEU:HD11	3:Y:30:ILE:HG12	1.89	0.54
3:X:26:VAL:O	3:X:30:ILE:HG13	2.08	0.54
2:C:898:GLY:C	2:C:900:ASN:H	2.10	0.54
2:D:814:LEU:HD12	2:D:814:LEU:N	2.22	0.54
3:X:50:LEU:HD12	3:X:67:LEU:HD23	1.88	0.54
1:A:23:ALA:CB	1:A:35:ALA:HB2	2.37	0.54
2:C:600:MET:O	2:C:630:ILE:HA	2.08	0.54
1:B:36:THR:HG22	1:B:51:PHE:HD2	1.73	0.54
3:Y:42:ARG:NH1	3:Y:72:ARG:HH21	2.06	0.54
2:D:931:TYR:CE1	2:D:940:LYS:HG2	2.43	0.54
1:A:40:PRO:CD	1:A:110:LEU:HD23	2.36	0.53
2:C:599:GLU:O	2:C:614:ARG:NH1	2.40	0.53
2:C:906:THR:HB	2:C:925:ARG:HG3	1.90	0.53
2:D:729:MET:O	2:D:729:MET:HG2	2.08	0.53
2:D:874:LYS:HD3	2:D:946:GLU:OE2	2.08	0.53
2:C:849:TYR:CE1	2:C:907:ILE:HD12	2.44	0.53
3:Y:1:MET:HB3	3:Y:17:VAL:O	2.08	0.53
2:C:584:PHE:CE1	2:C:819:LEU:HG	2.44	0.53
2:C:769:ASP:HB3	2:C:771:LYS:O	2.07	0.53
2:C:623:VAL:HG23	2:C:624:LEU:HD23	1.89	0.53
2:C:665:TYR:CE1	2:C:671:TYR:HA	2.44	0.53
2:C:910:TRP:HB3	2:C:927:ASP:HB3	1.91	0.53
2:D:783:ASN:HD22	2:D:783:ASN:C	2.11	0.53
2:D:942:LEU:C	2:D:944:ALA:H	2.12	0.53
1:A:94:SER:HB3	1:A:97:LEU:HG	1.91	0.53
1:A:72:ARG:HB2	1:A:145:TYR:CD2	2.44	0.53
1:A:142:THR:O	1:A:146:ALA:HB3	2.08	0.53
2:D:706:LEU:HD22	2:D:834:GLY:N	2.23	0.53
3:X:67:LEU:HD12	3:X:67:LEU:N	2.23	0.53
2:C:786:GLU:O	2:C:790:LEU:HG	2.09	0.52
2:D:687:LEU:O	2:D:691:THR:CG2	2.57	0.52
2:D:783:ASN:C	2:D:783:ASN:ND2	2.62	0.52
2:D:813:GLU:HB3	2:D:814:LEU:HD12	1.91	0.52
3:X:4:PHE:HD1	3:X:14:THR:HG22	1.74	0.52
1:A:86:LEU:HD13	1:A:109:LEU:HD22	1.91	0.52
2:D:729:MET:CE	2:D:795:ARG:HD2	2.38	0.52
1:B:129:THR:OG1	1:B:130:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:853:TYR:CD2	2:C:860:ILE:HD11	2.44	0.52
2:D:838:VAL:HG11	2:D:843:TRP:CE3	2.45	0.52
2:D:741:LYS:O	2:D:745:GLU:HG2	2.09	0.52
1:B:86:LEU:HD13	1:B:109:LEU:HD22	1.91	0.52
2:C:659:TYR:CG	2:D:597:ARG:HD3	2.45	0.52
1:A:70:THR:HG22	2:D:841:ASN:OD1	2.09	0.51
2:C:671:TYR:CZ	2:C:889:PRO:HG3	2.44	0.51
2:D:619:LYS:H	2:D:619:LYS:HE2	1.74	0.51
2:D:813:GLU:HB3	2:D:814:LEU:CD1	2.41	0.51
1:B:36:THR:HG22	1:B:51:PHE:CD2	2.45	0.51
2:C:830:LEU:HD23	2:C:830:LEU:O	2.11	0.51
3:X:15:LEU:HD13	3:X:29:LYS:HD3	1.92	0.51
1:B:119:LEU:O	2:D:925:ARG:NH2	2.43	0.51
2:C:857:HIS:HE1	2:C:859:VAL:HG23	1.75	0.51
2:C:863:PHE:O	2:C:867:VAL:HG23	2.11	0.51
2:D:686:HIS:CD2	2:D:687:LEU:N	2.76	0.51
2:D:729:MET:HG3	2:D:796:PHE:HZ	1.75	0.51
2:D:740:LEU:CD1	2:D:792:ILE:HD11	2.38	0.51
2:C:761:ASN:O	2:C:761:ASN:ND2	2.43	0.51
3:X:16:GLU:O	3:X:17:VAL:HG13	2.11	0.51
2:C:794:TRP:CD1	2:C:799:ARG:HD2	2.46	0.51
3:Y:1:MET:O	3:Y:2:GLN:HB2	2.11	0.51
2:C:640:TYR:HD2	2:C:640:TYR:N	2.09	0.51
2:C:676:ASN:OD1	2:C:678:ASN:N	2.43	0.51
2:C:740:LEU:HD22	2:C:788:ILE:HG23	1.93	0.50
2:D:606:ASN:HD22	2:D:610:GLU:HG3	1.76	0.50
2:D:914:GLU:HA	2:D:914:GLU:OE2	2.11	0.50
2:C:584:PHE:HE1	2:C:819:LEU:HG	1.75	0.50
3:Y:13:ILE:HG21	3:Y:34:GLU:OE2	2.11	0.50
1:B:122:GLU:O	1:B:126:ILE:HG12	2.11	0.50
2:D:817:ILE:HG23	2:D:818:ASP:N	2.25	0.50
1:A:41:ASN:ND2	1:A:46:GLN:OE1	2.45	0.50
1:A:15:ARG:HG2	1:A:15:ARG:NH2	2.26	0.50
2:D:786:GLU:O	2:D:790:LEU:HG	2.12	0.50
3:Y:26:VAL:O	3:Y:30:ILE:HG13	2.11	0.50
2:D:620:ARG:O	2:D:623:VAL:HG22	2.12	0.49
2:D:830:LEU:O	2:D:834:GLY:HA2	2.12	0.49
2:C:757:ILE:HD12	2:C:757:ILE:H	1.77	0.49
1:A:7:HIS:O	1:A:10:LEU:HB3	2.12	0.49
2:C:671:TYR:CE1	2:C:889:PRO:HD3	2.46	0.49
2:D:882:VAL:HG11	2:D:905:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:7:THR:HA	3:X:69:LEU:HB3	1.94	0.49
2:C:929:PRO:HG2	2:C:931:TYR:CZ	2.47	0.49
1:A:75:HIS:HE1	1:A:77:ASN:OD1	1.95	0.49
2:C:640:TYR:N	2:C:640:TYR:CD2	2.81	0.49
2:D:583:TYR:CE1	2:D:587:LYS:HG2	2.47	0.49
1:B:63:LYS:HB3	1:B:63:LYS:HZ2	1.76	0.49
2:C:583:TYR:O	2:C:587:LYS:HG3	2.12	0.49
2:C:949:GLN:O	2:C:949:GLN:HG2	2.13	0.49
3:Y:17:VAL:HG12	3:Y:29:LYS:HZ2	1.78	0.49
1:B:117:ASP:O	3:Y:76:GLY:O	2.31	0.49
2:D:604:ARG:HG2	2:D:604:ARG:HH11	1.78	0.49
1:A:45:TYR:CE2	1:A:138:ALA:HB1	2.48	0.49
2:D:601:LYS:NZ	2:D:633:GLU:HG2	2.28	0.49
1:A:74:TYR:HB2	1:A:141:TRP:CD2	2.48	0.48
2:C:671:TYR:CE2	2:C:889:PRO:HG3	2.47	0.48
2:C:761:ASN:O	2:C:764:GLN:HB2	2.13	0.48
2:D:787:TYR:O	2:D:790:LEU:N	2.46	0.48
3:Y:44:ILE:HD13	3:Y:49:GLN:HA	1.95	0.48
2:C:699:LEU:N	2:C:814:LEU:HD13	2.28	0.48
1:B:121:PRO:HG2	1:B:122:GLU:H	1.78	0.48
2:C:756:CYS:SG	2:C:775:SER:HA	2.54	0.48
1:B:136:ARG:O	1:B:140:GLU:HG3	2.14	0.48
2:C:699:LEU:CA	2:C:814:LEU:HD13	2.42	0.48
3:Y:23:ILE:HB	3:Y:51:GLU:O	2.13	0.48
1:B:13:LEU:CD2	1:B:18:PRO:HD3	2.43	0.48
2:C:760:GLU:HA	2:C:764:GLN:O	2.13	0.48
3:X:54:ARG:HG2	3:X:54:ARG:HH11	1.77	0.48
2:D:697:ALA:HA	2:D:707:LEU:HD21	1.95	0.48
3:X:13:ILE:HD11	3:X:34:GLU:HG3	1.96	0.48
1:A:19:ALA:HB1	1:A:20:GLN:HE21	1.79	0.48
2:C:695:ARG:O	2:C:814:LEU:CD1	2.61	0.48
2:D:888:VAL:HG13	2:D:889:PRO:HD2	1.95	0.48
3:Y:17:VAL:CG1	3:Y:29:LYS:HZ3	2.26	0.48
1:A:25:PRO:HA	1:A:33:TRP:HA	1.96	0.47
2:C:737:TYR:CZ	2:C:741:LYS:HD3	2.49	0.47
2:C:632:PHE:C	2:C:634:SER:H	2.17	0.47
2:C:812:THR:CG2	2:C:817:ILE:HB	2.44	0.47
2:D:701:VAL:HG13	2:D:831:LEU:HD11	1.96	0.47
2:C:743:ILE:CD1	2:C:751:LEU:CD1	2.93	0.47
2:D:941:LEU:O	2:D:945:VAL:HG23	2.15	0.47
2:C:918:ARG:HG2	2:C:918:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:928:LEU:HD12	2:C:929:PRO:HD2	1.97	0.47
2:D:710:PHE:CE1	2:D:833:CYS:HB2	2.50	0.47
2:C:638:LEU:HG	2:C:638:LEU:O	2.14	0.47
2:C:820:ILE:HD11	2:C:828:LEU:CD1	2.44	0.47
2:D:757:ILE:HD13	2:D:758:ASP:H	1.80	0.47
3:X:15:LEU:HD22	3:X:29:LYS:CE	2.43	0.47
2:C:597:ARG:HA	2:C:627:ARG:H	1.80	0.47
2:C:637:GLY:O	2:C:640:TYR:HE2	1.97	0.47
2:C:686:HIS:CD2	2:C:687:LEU:HG	2.50	0.47
2:C:863:PHE:O	2:C:866:ALA:HB3	2.15	0.47
2:C:918:ARG:HG2	2:C:918:ARG:NH1	2.30	0.47
2:C:937:LEU:C	2:C:937:LEU:HD23	2.35	0.47
1:A:111:CYS:C	1:A:113:PRO:HD3	2.36	0.47
1:B:88:ILE:O	1:B:93:TRP:HB2	2.15	0.47
2:C:606:ASN:O	2:C:610:GLU:HG3	2.15	0.47
3:Y:42:ARG:NH2	3:Y:49:GLN:OE1	2.48	0.47
2:D:854:CYS:HB2	2:D:855:PRO:HD2	1.97	0.47
1:B:54:ILE:HG12	1:B:67:VAL:HG22	1.98	0.46
2:D:729:MET:HG3	2:D:796:PHE:CZ	2.50	0.46
3:X:13:ILE:HG23	3:X:33:LYS:CD	2.43	0.46
3:X:45:PHE:CE1	3:X:65:SER:HB3	2.51	0.46
2:C:604:ARG:NH2	2:C:635:GLU:HB2	2.29	0.46
3:X:24:GLU:HB2	3:X:52:ASP:HB3	1.96	0.46
1:B:95:PRO:HG3	2:D:739:SER:HB3	1.97	0.46
2:C:686:HIS:CD2	2:C:687:LEU:N	2.82	0.46
2:D:771:LYS:NZ	2:D:786:GLU:OE2	2.49	0.46
1:A:147:MET:O	2:D:844:ARG:HD2	2.15	0.46
2:C:597:ARG:HD2	2:C:629:TRP:CE3	2.50	0.46
2:C:747:ASP:CG	2:C:781:ASN:HD22	2.19	0.46
2:D:671:TYR:CE2	2:D:889:PRO:HG3	2.50	0.46
2:D:757:ILE:HD13	2:D:758:ASP:N	2.30	0.46
3:X:54:ARG:HG2	3:X:54:ARG:NH1	2.31	0.46
1:A:8:LYS:HE2	2:C:752:ASP:HB2	1.97	0.46
2:C:741:LYS:O	2:C:744:LEU:HB3	2.16	0.46
3:X:50:LEU:CD1	3:X:67:LEU:HD23	2.45	0.46
2:D:793:GLN:NE2	2:D:798:ASN:OD1	2.48	0.46
1:A:19:ALA:O	1:A:20:GLN:HB2	2.15	0.46
1:A:64:PRO:HB3	1:A:93:TRP:CG	2.50	0.46
2:D:583:TYR:O	2:D:587:LYS:HB2	2.16	0.46
1:A:72:ARG:HB2	1:A:145:TYR:CG	2.50	0.46
1:B:60:TYR:CD1	1:B:61:PRO:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ARG:HG3	1:B:72:ARG:NH1	2.31	0.46
2:D:597:ARG:NH1	2:D:597:ARG:CG	2.74	0.46
2:D:601:LYS:HZ3	2:D:639:ASP:CB	2.29	0.46
2:D:697:ALA:CB	2:D:707:LEU:HD11	2.47	0.46
2:C:685:ASP:N	2:C:685:ASP:OD1	2.48	0.45
2:C:948:ALA:O	2:C:949:GLN:HB3	2.17	0.45
2:D:781:ASN:O	2:D:781:ASN:ND2	2.49	0.45
1:B:37:ILE:HD12	1:B:52:LEU:HD11	1.99	0.45
2:C:620:ARG:HH11	2:C:620:ARG:HB2	1.82	0.45
2:D:917:PRO:O	3:Y:73:LEU:HD22	2.16	0.45
2:D:814:LEU:N	2:D:814:LEU:CD1	2.79	0.45
2:C:891:ASN:HB2	2:C:895:GLU:HG3	1.98	0.45
2:D:716:TYR:CZ	2:D:829:GLU:HG3	2.52	0.45
2:C:683:ASN:C	2:C:685:ASP:H	2.20	0.45
2:C:690:PHE:CE2	2:C:803:GLN:HG2	2.52	0.45
2:C:820:ILE:HG12	2:C:820:ILE:O	2.16	0.45
1:A:37:ILE:HG13	1:A:52:LEU:HD11	1.98	0.45
2:C:747:ASP:HA	2:C:781:ASN:ND2	2.32	0.45
2:D:673:LEU:O	2:D:711:PHE:HA	2.17	0.45
2:D:748:PRO:O	2:D:749:THR:C	2.55	0.45
3:X:13:ILE:HG22	3:X:15:LEU:HG	1.98	0.45
2:C:697:ALA:HA	2:C:707:LEU:HD11	1.98	0.45
2:D:601:LYS:HZ3	2:D:639:ASP:HB3	1.82	0.45
2:D:653:LYS:O	2:D:657:ASN:HB2	2.17	0.45
1:B:117:ASP:N	1:B:118:PRO:CD	2.78	0.45
2:C:608:PHE:HE2	2:C:689:TYR:CE2	2.35	0.45
2:D:836:GLY:O	2:D:876:ILE:HD11	2.16	0.45
2:D:888:VAL:CG1	2:D:889:PRO:HD2	2.47	0.45
1:A:88:ILE:O	1:A:93:TRP:HB2	2.16	0.45
2:D:601:LYS:NZ	2:D:639:ASP:HB3	2.32	0.45
3:Y:17:VAL:CG1	3:Y:29:LYS:NZ	2.80	0.45
1:A:51:PHE:CD2	2:D:868:LEU:HD11	2.51	0.45
1:A:75:HIS:ND1	1:A:76:PRO:N	2.65	0.45
1:B:35:ALA:O	1:B:51:PHE:HA	2.17	0.45
1:A:9:GLU:OE1	1:A:98:LYS:HA	2.16	0.44
2:D:918:ARG:HH22	3:Y:75:GLY:HA3	1.82	0.44
1:A:50:PHE:CE1	1:A:73:ILE:HD12	2.51	0.44
1:B:79:ASN:ND2	1:B:83:SER:HB2	2.33	0.44
1:B:113:PRO:C	1:B:115:PRO:HD3	2.38	0.44
2:C:675:ILE:N	2:C:675:ILE:CD1	2.74	0.44
2:C:807:PHE:CD2	2:C:807:PHE:C	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:869:LEU:HD13	2:D:938:ARG:NH1	2.33	0.44
2:D:880:GLN:O	2:D:881:PHE:C	2.56	0.44
2:C:764:GLN:HE21	2:C:764:GLN:CA	2.27	0.44
3:X:16:GLU:H	3:X:29:LYS:HE2	1.83	0.44
1:A:75:HIS:ND1	1:A:76:PRO:CD	2.80	0.44
2:C:645:ARG:HH11	2:C:705:LYS:CD	2.31	0.44
2:C:696:VAL:O	2:C:699:LEU:HB3	2.18	0.44
2:C:759:GLU:HB2	2:C:766:TYR:CE1	2.53	0.44
2:D:835:LEU:HD23	2:D:836:GLY:H	1.82	0.44
1:B:36:THR:HA	1:B:50:PHE:O	2.18	0.44
1:A:6:ILE:HG23	1:A:33:TRP:CZ2	2.53	0.44
1:B:117:ASP:N	1:B:118:PRO:HD3	2.33	0.44
2:C:648:PHE:CE2	2:C:705:LYS:HG3	2.53	0.44
2:C:756:CYS:HB2	2:C:768:VAL:O	2.18	0.44
2:D:612:TYR:CE1	2:D:616:MET:HG3	2.53	0.44
2:D:635:GLU:H	2:D:635:GLU:HG3	1.61	0.43
1:A:111:CYS:O	1:A:113:PRO:HD3	2.18	0.43
2:C:669:ASP:OD1	2:C:669:ASP:N	2.51	0.43
2:C:898:GLY:C	2:C:900:ASN:N	2.71	0.43
2:C:911:GLY:O	2:C:930:PRO:HD2	2.18	0.43
2:C:912:SER:OG	2:C:914:GLU:CG	2.66	0.43
2:D:949:GLN:OE1	2:D:949:GLN:N	2.39	0.43
1:A:58:THR:HG21	2:C:760:GLU:HG3	2.00	0.43
2:C:598:PHE:N	2:C:627:ARG:O	2.44	0.43
3:Y:41:GLN:HB2	3:Y:69:LEU:CD1	2.38	0.43
2:D:899:SER:C	2:D:900:ASN:HD22	2.22	0.43
2:C:923:PHE:O	2:C:924:ASN:C	2.57	0.43
2:D:662:LEU:HA	2:D:662:LEU:HD23	1.86	0.43
2:D:921:THR:HG23	3:Y:74:ARG:CD	2.48	0.43
1:A:90:ARG:HG2	1:A:90:ARG:NH1	2.31	0.43
2:C:651:LEU:O	2:C:655:MET:HG3	2.19	0.43
2:D:863:PHE:O	2:D:867:VAL:HG23	2.19	0.43
2:D:876:ILE:CG2	2:D:886:SER:HB2	2.49	0.43
2:C:929:PRO:HG2	2:C:931:TYR:CE2	2.53	0.43
2:D:632:PHE:O	2:D:639:ASP:HA	2.18	0.43
1:A:74:TYR:HB2	1:A:141:TRP:CE3	2.54	0.43
2:C:620:ARG:NH1	2:C:620:ARG:CB	2.82	0.43
2:C:658:PRO:HA	2:C:663:PHE:O	2.19	0.43
1:A:37:ILE:HG13	1:A:52:LEU:CD1	2.49	0.43
1:A:74:TYR:CE1	1:A:123:ILE:HG23	2.54	0.43
2:C:857:HIS:CE1	2:C:859:VAL:HG23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:948:ALA:O	3:X:8:LEU:HD23	2.19	0.43
2:D:947:ASN:HA	3:Y:8:LEU:HD23	2.00	0.43
3:Y:22:THR:HA	3:Y:55:THR:HA	2.00	0.43
2:C:789:ASP:O	2:C:793:GLN:HB2	2.19	0.42
2:D:947:ASN:CB	3:Y:71:LEU:HD12	2.45	0.42
1:B:87:ASP:HB3	1:B:92:GLN:HB2	2.00	0.42
1:B:5:ARG:NH1	1:B:97:LEU:O	2.53	0.42
1:B:139:ARG:O	1:B:143:GLN:HB2	2.20	0.42
2:C:607:ILE:HD13	2:C:650:LEU:HB3	2.01	0.42
2:D:816:PRO:HG2	2:D:819:LEU:HB2	2.01	0.42
2:D:910:TRP:CG	2:D:911:GLY:N	2.87	0.42
2:C:713:ARG:HH21	2:C:717:LYS:HD2	1.84	0.42
2:D:716:TYR:CE2	2:D:829:GLU:HG3	2.54	0.42
1:B:72:ARG:HG3	1:B:72:ARG:HH11	1.84	0.42
1:B:15:ARG:HD3	1:B:15:ARG:C	2.40	0.42
2:D:784:LYS:O	2:D:788:ILE:HG13	2.20	0.42
3:Y:28:ALA:O	3:Y:32:ASP:OD1	2.38	0.42
3:Y:49:GLN:O	3:Y:49:GLN:HG3	2.19	0.42
2:D:600:MET:HG2	2:D:614:ARG:HG2	2.02	0.42
2:C:942:LEU:O	2:C:946:GLU:HG2	2.20	0.42
2:D:758:ASP:OD2	2:D:767:GLN:HG3	2.19	0.42
2:D:880:GLN:HA	2:D:885:THR:O	2.20	0.42
2:C:673:LEU:O	2:C:711:PHE:HA	2.19	0.42
2:C:761:ASN:N	2:C:761:ASN:ND2	2.65	0.42
2:C:576:GLU:O	2:C:577:PHE:C	2.58	0.41
2:C:851:ASN:ND2	2:C:909:GLN:O	2.53	0.41
2:C:921:THR:HG21	3:X:74:ARG:NH1	2.35	0.41
2:D:604:ARG:HH11	2:D:604:ARG:CG	2.32	0.41
2:D:910:TRP:O	2:D:929:PRO:HA	2.20	0.41
1:B:3:SER:O	1:B:7:HIS:HB2	2.20	0.41
3:Y:63:LYS:O	3:Y:64:GLU:HB2	2.21	0.41
2:D:607:ILE:HG23	2:D:608:PHE:N	2.35	0.41
1:A:26:VAL:HG23	1:A:34:GLN:HG2	2.01	0.41
1:B:126:ILE:HD12	1:B:133:LYS:HZ2	1.83	0.41
2:C:620:ARG:HH11	2:C:623:VAL:HG13	1.85	0.41
2:D:866:ALA:O	2:D:870:MET:HG2	2.20	0.41
1:B:134:TYR:O	1:B:135:ASN:C	2.59	0.41
2:D:942:LEU:C	2:D:944:ALA:N	2.73	0.41
2:D:670:ASN:O	2:D:671:TYR:HB2	2.20	0.41
3:X:22:THR:O	3:X:23:ILE:C	2.59	0.41
1:B:66:LYS:HD2	1:B:66:LYS:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:757:ILE:H	2:C:757:ILE:CD1	2.33	0.41
2:C:854:CYS:HB2	2:C:855:PRO:HD2	2.03	0.41
2:D:596:ASN:HD22	2:D:596:ASN:HA	1.62	0.41
2:D:621:PRO:O	2:D:624:LEU:HD12	2.21	0.41
3:Y:14:THR:HG22	3:Y:15:LEU:N	2.35	0.41
1:B:59:ASP:HB2	1:B:63:LYS:HG3	2.02	0.41
2:C:814:LEU:HB2	2:C:815:LEU:HD12	2.03	0.41
1:A:42:ASP:HA	1:A:46:GLN:NE2	2.35	0.41
1:B:5:ARG:HG2	1:B:61:PRO:HG3	2.03	0.41
1:B:128:LYS:HA	1:B:128:LYS:HD3	1.71	0.41
2:C:653:LYS:HD3	2:C:890:MET:HG3	2.03	0.41
2:C:762:PHE:C	2:C:764:GLN:H	2.23	0.41
2:C:815:LEU:HA	2:C:816:PRO:HD3	1.80	0.41
2:C:894:ALA:HB1	2:D:640:TYR:HA	2.03	0.41
2:C:933:THR:OG1	2:C:936:ASP:CB	2.67	0.41
3:Y:72:ARG:O	3:Y:72:ARG:HG3	2.20	0.41
1:A:126:ILE:O	1:A:130:ASP:O	2.39	0.41
2:C:771:LYS:HB2	2:C:772:PRO:HD2	2.03	0.41
2:D:619:LYS:HE3	2:D:619:LYS:N	2.29	0.41
2:D:937:LEU:HD23	2:D:938:ARG:N	2.36	0.41
1:A:25:PRO:HB3	1:A:33:TRP:CD1	2.56	0.40
2:C:608:PHE:CE1	2:C:655:MET:HG2	2.56	0.40
2:C:921:THR:CG2	3:X:74:ARG:HH11	2.34	0.40
2:D:914:GLU:OE2	2:D:914:GLU:CA	2.69	0.40
1:B:79:ASN:HD21	1:B:83:SER:HB2	1.85	0.40
2:C:740:LEU:HA	2:C:740:LEU:HD23	1.89	0.40
2:D:766:TYR:N	2:D:766:TYR:CD1	2.89	0.40
2:D:789:ASP:O	2:D:793:GLN:HB2	2.22	0.40
3:X:45:PHE:CB	3:X:50:LEU:HD21	2.45	0.40
1:B:126:ILE:O	1:B:130:ASP:O	2.39	0.40
2:C:691:THR:HA	2:C:806:ALA:O	2.21	0.40
2:C:692:PHE:O	2:C:695:ARG:N	2.55	0.40
2:D:670:ASN:O	2:D:671:TYR:CB	2.69	0.40
2:D:937:LEU:HD23	2:D:937:LEU:C	2.42	0.40
3:Y:5:VAL:HA	3:Y:67:LEU:O	2.20	0.40
3:Y:7:THR:CG2	3:Y:69:LEU:HD23	2.52	0.40
1:A:137:ILE:O	1:A:138:ALA:C	2.60	0.40
1:B:15:ARG:HD3	1:B:16:ASP:HB2	2.03	0.40
1:B:56:PHE:HZ	1:B:99:ILE:HG13	1.87	0.40
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.88	0.40
2:D:594:ILE:HB	2:D:595:PRO:HD2	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%)	133 (92%)	10 (7%)	1 (1%)	22	54
1	B	144/146 (99%)	124 (86%)	17 (12%)	3 (2%)	7	31
2	C	375/385 (97%)	321 (86%)	50 (13%)	4 (1%)	14	45
2	D	372/385 (97%)	328 (88%)	42 (11%)	2 (0%)	29	61
3	X	74/81 (91%)	64 (86%)	8 (11%)	2 (3%)	5	26
3	Y	74/81 (91%)	63 (85%)	9 (12%)	2 (3%)	5	26
All	All	1183/1224 (97%)	1033 (87%)	136 (12%)	14 (1%)	13	42

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	SER
2	D	825	GLU
1	B	129	THR
2	C	593	ASP
3	Y	2	GLN
3	Y	21	ASP
2	C	949	GLN
3	X	51	GLU
2	C	798	ASN
2	C	595	PRO
1	A	113	PRO
2	D	658	PRO
3	X	23	ILE
1	B	126	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/130 (100%)	123 (95%)	7 (5%)	22	53
1	B	130/130 (100%)	118 (91%)	12 (9%)	9	31
2	C	341/347 (98%)	315 (92%)	26 (8%)	13	39
2	D	339/347 (98%)	306 (90%)	33 (10%)	8	29
3	X	68/70 (97%)	64 (94%)	4 (6%)	19	49
3	Y	68/70 (97%)	64 (94%)	4 (6%)	19	49
All	All	1076/1094 (98%)	990 (92%)	86 (8%)	12	37

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	41	ASN
1	A	66	LYS
1	A	91	SER
1	A	98	LYS
1	A	114	ASN
1	A	130	ASP
1	B	3	SER
1	B	15	ARG
1	B	34	GLN
1	B	42	ASP
1	B	58	THR
1	B	66	LYS
1	B	72	ARG
1	B	85	SER
1	B	87	ASP
1	B	92	GLN
1	B	118	PRO
1	B	143	GLN
2	C	586	LYS
2	C	596	ASN
2	C	601	LYS

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Mol	Chain	Res	Type
2	C	602	LEU
2	C	614	ARG
2	C	622	ASP
2	C	628	LEU
2	C	640	TYR
2	C	650	LEU
2	C	668	THR
2	C	675	ILE
2	C	686	HIS
2	C	757	ILE
2	C	761	ASN
2	C	764	GLN
2	C	767	GLN
2	C	772	PRO
2	C	805	ASN
2	C	822	ILE
2	C	841	ASN
2	C	856	ASN
2	C	887	ARG
2	C	896	LEU
2	C	906	THR
2	C	932	GLU
2	C	943	MET
2	D	587	LYS
2	D	597	ARG
2	D	602	LEU
2	D	604	ARG
2	D	614	ARG
2	D	619	LYS
2	D	622	ASP
2	D	628	LEU
2	D	635	GLU
2	D	638	LEU
2	D	658	PRO
2	D	668	THR
2	D	670	ASN
2	D	686	HIS
2	D	691	THR
2	D	713	ARG
2	D	725	THR
2	D	727	ASN
2	D	757	ILE

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Mol	Chain	Res	Type
2	D	769	ASP
2	D	771	LYS
2	D	772	PRO
2	D	783	ASN
2	D	801	GLN
2	D	802	LYS
2	D	818	ASP
2	D	835	LEU
2	D	841	ASN
2	D	877	ARG
2	D	893	PHE
2	D	896	LEU
2	D	913	PRO
2	D	932	GLU
3	X	58	ASP
3	X	64	GLU
3	X	67	LEU
3	X	72	ARG
3	Y	32	ASP
3	Y	52	ASP
3	Y	58	ASP
3	Y	64	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	20	GLN
1	A	32	HIS
1	A	41	ASN
1	A	46	GLN
1	A	55	HIS
1	B	11	ASN
1	B	55	HIS
1	B	143	GLN
2	C	683	ASN
2	C	761	ASN
2	C	764	GLN
2	C	781	ASN
2	C	793	GLN
2	C	798	ASN
2	C	856	ASN

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Mol	Chain	Res	Type
2	C	891	ASN
2	C	909	GLN
2	C	947	ASN
2	D	596	ASN
2	D	606	ASN
2	D	670	ASN
2	D	727	ASN
2	D	767	GLN
2	D	783	ASN
2	D	793	GLN
2	D	798	ASN
2	D	801	GLN
2	D	805	ASN
2	D	900	ASN
2	D	909	GLN
3	X	62	GLN
3	Y	2	GLN
3	Y	25	ASN
3	Y	41	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	146/146 (100%)	0.08	0	100	100	35, 80, 104, 114	0
1	B	146/146 (100%)	0.13	0	100	100	52, 77, 99, 114	0
2	C	377/385 (97%)	0.01	3 (0%)	86	86	45, 72, 112, 122	0
2	D	374/385 (97%)	-0.05	0	100	100	38, 67, 96, 126	0
3	X	76/81 (93%)	1.19	23 (30%)	0	0	93, 126, 127, 127	0
3	Y	76/81 (93%)	1.38	20 (26%)	0	0	95, 125, 127, 127	0
All	All	1195/1224 (97%)	0.18	46 (3%)	40	37	35, 75, 126, 127	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	1	MET	5.1
3	Y	15	LEU	4.1
3	Y	66	THR	4.0
3	Y	43	LEU	4.0
3	X	2	GLN	3.5
3	Y	34	GLU	3.5
3	X	66	THR	3.3
3	Y	17	VAL	3.3
3	X	12	THR	3.0
3	Y	16	GLU	2.8
3	X	22	THR	2.8
3	X	3	ILE	2.8
3	X	51	GLU	2.7
3	Y	22	THR	2.7
3	X	15	LEU	2.6
3	X	65	SER	2.6
3	Y	3	ILE	2.6
3	Y	50	LEU	2.6
3	Y	59	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	X	11	LYS	2.5
3	X	9	THR	2.5
3	Y	2	GLN	2.5
3	Y	36	ILE	2.4
3	X	16	GLU	2.4
3	X	10	GLY	2.4
3	X	17	VAL	2.3
3	X	61	ILE	2.3
3	X	49	GLN	2.3
3	Y	49	GLN	2.3
3	Y	13	ILE	2.3
3	Y	21	ASP	2.3
3	X	21	ASP	2.3
3	Y	30	ILE	2.3
3	Y	54	ARG	2.3
3	X	59	TYR	2.3
2	C	619	LYS	2.2
3	X	63	LYS	2.2
2	C	624	LEU	2.2
3	Y	65	SER	2.1
3	X	50	LEU	2.1
3	X	64	GLU	2.1
3	Y	35	GLY	2.1
3	Y	64	GLU	2.1
3	X	23	ILE	2.0
3	X	30	ILE	2.0
2	C	639	ASP	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.