



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:50 AM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

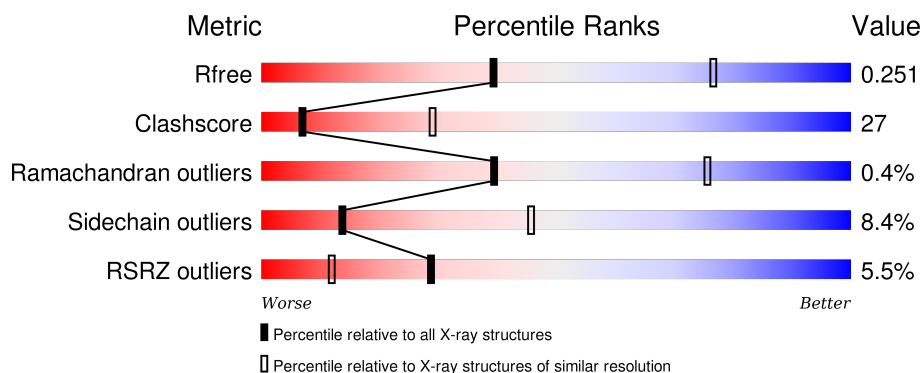
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>2%</div> <div>54%</div> <div>44%</div> <div>•</div> </div>
1	B	146	<div> <div>%</div> <div>53%</div> <div>40%</div> <div>7%</div> </div>
2	C	385	<div> <div>%</div> <div>49%</div> <div>45%</div> <div>• •</div> </div>
2	D	385	<div> <div>55%</div> <div>37%</div> <div>5%</div> <div>•</div> </div>
3	X	81	<div> <div>38%</div> <div>40%</div> <div>53%</div> <div>• 6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Y	81	<div><div><div></div><div></div><div></div><div></div></div><div>33%46%46%6%</div></div>

## 2 Entry composition

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
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	UNP P62837
A	85	SER	CYS	ENGINEERED	UNP P62837
A	98	LYS	THR	ENGINEERED	UNP P62837
B	3	SER	LEU	ENGINEERED	UNP P62837
B	85	SER	CYS	ENGINEERED	UNP P62837
B	98	LYS	THR	ENGINEERED	UNP P62837

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	376	Total	C	N	O	S	0	0	0
			3140	2032	519	572	17			
2	D	374	Total	C	N	O	S	0	0	0
			3125	2021	517	570	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	SER	CYS	ENGINEERED	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	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 4 is water.

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:
- 
- 54% 44% 2%
- Q92 W93 A96 I99 S100 K101 V102 I106 L110 C111 D116 D117 P118 P121 E122 I123 D130 R131 E132 K133 Y134 N135 R136 E140 W141 T142 Y145 A146 M147
- A2 R5 I6 H7 K8 E9 L10 M11 D12 I13 A14 R15 P17 P18 A19 Q20 C21 S22 P25 V26 D29 F30 F31 H32 H33 Q34 A35 T36 G39 P40 H41 Y45 F50 F51 T58 D59 V60 P61 P62 K63 P64 R72 I73 V74 H75 P76 R77 I88 S91

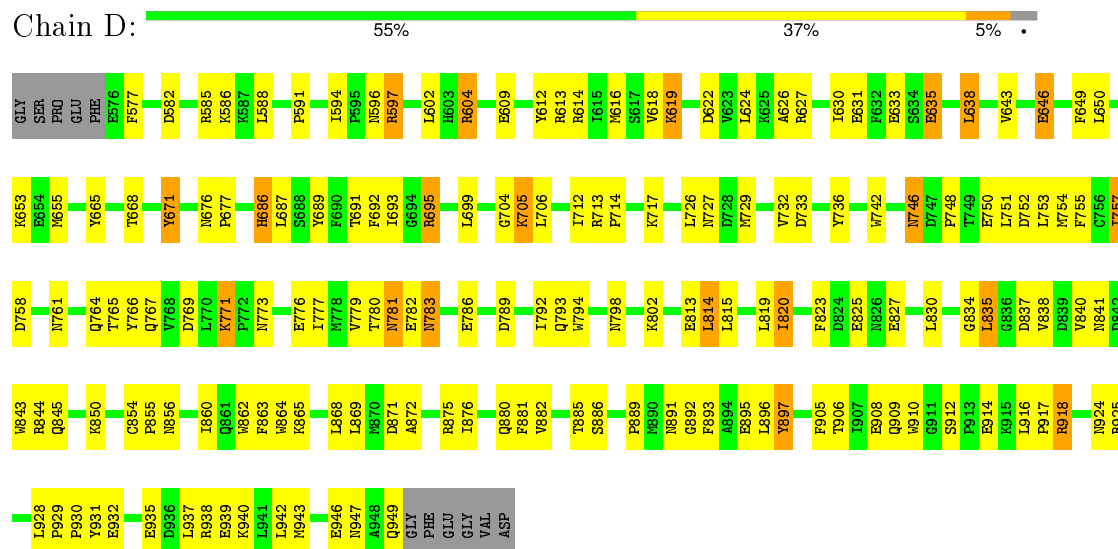
- Chain B:
- 
- 53% 40% 7%
- A2 S3 K4 R5 I6 H7 K8 E9 L10 M11 D12 L13 A14 R15 D16 P17 H18 A19 Q20 D21 M23 Q24 A25 T36 I37 D42 S43 P44 F50 F51 L52 T53 I54 H55 Y60 P61 K66 V67 A68 F69 H75 P76 N79 G82 S83 I84 S85 L86 D87 I88 I89 R90 S91 Q92 K98 I99 S100 K101 S105 P113 M114 P115 D116 D117 P118 P121 E122 I123 I126 Y127 K128 T129 D130 R131 F132 K133 Y134 N135 A138 R139 T142 Q143 K144 Y145 A146 M147

- Chain C: 

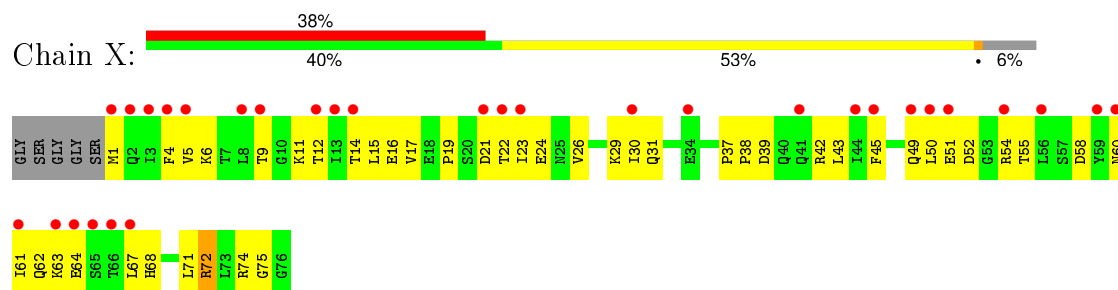
Category	Value
L814	7173
L815	6636
L816	6637
L817	6638
L818	6639
L819	6640
L820	6643
L821	6644
L822	6645
L823	6646
L824	6647
L825	6648
L826	6649
L827	6650
L828	6651
L829	6652
L830	6653
L831	6654
L832	6655
L833	6656
L834	6657
L835	6658
L836	6659
L837	6660
L838	6661
L839	6662
L840	6663
L841	6664
L842	6665
L843	6666
L844	6667
L845	6668
L846	6669
L847	6670
L848	6671
L849	6672
L850	6673
L851	6674
L852	6675
L853	6676
L854	6677
L855	6678
L856	6679
L857	6680
L858	6681
L859	6682
L860	6683
L861	6684
L862	6685
L863	6686
L864	6687
L865	6688
L866	6689
L867	6690
L868	6691
L869	6692
L870	6693
L871	6694
L872	6695
L873	6696
L874	6697
L875	6698
L876	6699
L877	6700
L878	6701
L879	6702
L880	6703
L881	6704
L882	6705
L883	6706
L884	6707
L885	6708
L886	6709
L887	6710
L888	6711
L889	6712
L890	6713
L891	6714
L892	6715
L893	6716
L894	6717
L895	6718
L896	6719
L897	6720
L898	6721
L899	6722
L900	6723
L901	6724
L902	6725
L903	6726
L904	6727
L905	6728
L906	6729
L907	6730
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L911	6734
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L914	6737
L915	6738
L916	6739
L917	6740
L918	6741
L919	6742
L920	6743
L921	6744
L922	6745
L923	6746
L924	6747
L925	6748
L926	6749
L927	6750
L928	6751
L929	6752
L930	6753
L931	6754
L932	6755
L933	6756
L934	6757
L935	6758
L936	6759
L937	6760
L938	6761
L939	6762
L940	6763
L941	6764
L942	6765
L943	6766
L944	6767
L945	6768
L946	6769
L947	6770
L948	6771
L949	6772
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L952	6775
L953	6776
L954	6777
L955	6778
L956	6779
L957	6780
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L959	6782
L960	6783
L961	6784
L962	6785
L963	6786
L964	6787
L965	6788
L966	6789
L967	6790
L968	6791
L969	6792
L970	6793
L971	6794
L972	6795
L973	6796
L974	6797
L975	6798
L976	6799
L977	6800
L978	6801
L979	6802
L980	6803
L981	6804
L982	6805
L983	6806
L984	6807
L985	6808
L986	6809
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L990	6813
L991	6814
L992	6815
L993	6816
L994	6817



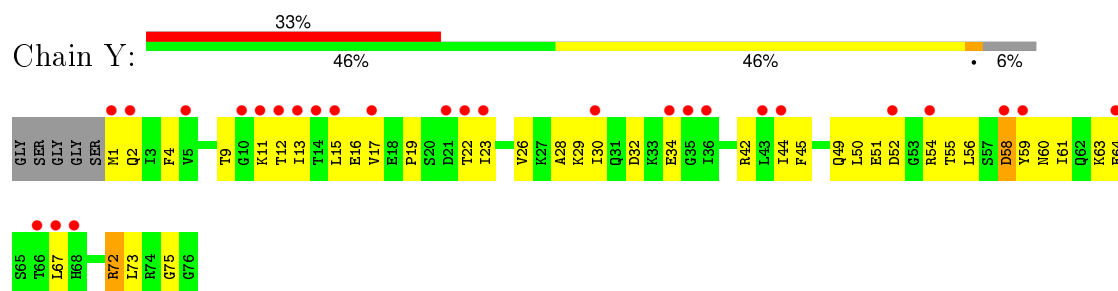
• Molecule 2: E3 ubiquitin-protein ligase NEDD4-like



• 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.46 (at 3.12Å)	Xtriage
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%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.9	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 61.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 33799 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	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

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:H	2:D:619:LYS:HE3	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:813:GLU:HB3	2:D:814:LEU:HD12	1.63	0.80
2:D:646:GLU:HG3	2:D:650:LEU:CD1	2.12	0.80
2:D:619:LYS:N	2:D:619:LYS:HE3	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:910:TRP:CZ3	2:D:918:ARG:HD2	2.20	0.76
2:D:604:ARG:CG	2:D:604:ARG:HH11	1.99	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
2:D:918:ARG:HH12	3:Y:75:GLY:HA2	1.52	0.74
1:A:58:THR:HG21	2:C:760:GLU:HG3	1.69	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
3:X:45:PHE:HB3	3:X:50:LEU:HD21	1.72	0.71
2:D:943:MET:O	2:D:947:ASN:ND2	2.22	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:794:TRP:HA	2:C:798:ASN:HD22	1.57	0.69
2:C:637:GLY:O	2:C:640:TYR:HE2	1.74	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:H	2:D:638:LEU:CD2	2.07	0.68
2:D:794:TRP:HA	2:D:798:ASN:ND2	2.09	0.68
2:C:656:PHE:HB3	2:C:673:LEU:HD13	1.75	0.68
2:C:874:LYS:HD2	2:C:874:LYS:H	1.57	0.67
2:D:781:ASN:O	2:D:781:ASN:ND2	2.28	0.67
2:D:726:LEU:HA	2:D:792:ILE:HD13	1.77	0.67
2:C:667:ALA:HB3	2:C:670:ASN:HB2	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:HG2	3:X:31:GLN:O	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:N	2:C:640:TYR:HD2	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:O	2:D:830:LEU:HG	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
2:D:619:LYS:H	2:D:619:LYS:CE	2.10	0.64
2:D:862:TRP:O	2:D:865:LYS:HB3	1.97	0.64
2:C:726:LEU:HA	2:C:792:ILE:HD11	1.79	0.64
2:D:704:GLY:O	2:D:705:LYS:HE2	1.97	0.64
1:A:72:ARG:HG3	1:A:72:ARG:HH11	1.61	0.64
2:C:757:ILE:HG22	2:C:758:ASP:N	2.13	0.64
2:C:601:LYS:HA	2:C:631:GLU:O	1.98	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:814:LEU:N	2:D:814:LEU:HD12	2.13	0.63
2:D:646:GLU:HG3	2:D:650:LEU:HD13	1.79	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
2:D:910:TRP:CH2	2:D:918:ARG:HD2	2.34	0.63
1:B:144:LYS:HD2	1:B:145:TYR:CZ	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
3:X:45:PHE:HB2	3:X:50:LEU:HD11	1.80	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
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:HD22	1:B:11:ASN:N	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:D:863:PHE:HA	2:D:937:LEU:HD21	1.83	0.59
2:C:645:ARG:NH1	2:C:705:LYS:HE2	2.18	0.59
2:D:779:VAL:HG23	2:D:779:VAL:O	2.03	0.59
1:B:56:PHE:CE2	1:B:99:ILE:HD11	2.38	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
3:X:23:ILE:HA	3:X:26:VAL:HG23	1.84	0.58
2:D:891:ASN:HD22	2:D:895:GLU:HG3	1.68	0.58
2:D:604:ARG:HG2	2:D:604:ARG:HH11	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: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
2:D:686:HIS:CD2	2:D:687:LEU:H	2.21	0.58
1:B:13:LEU:HD23	1:B:18:PRO:HD2	1.85	0.58
2:D:815:LEU:HD23	2:D:820:ILE:CD1	2.33	0.57
2:C:665:TYR:CD1	2:C:671:TYR:HA	2.38	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
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:A:142:THR:O	1:A:147:MET:HG3	2.04	0.57
2:D:650:LEU:N	2:D:650:LEU:HD12	2.20	0.57
3:X:31:GLN:HE21	3:X:38:PRO:HD3	1.67	0.57
1:B:55:HIS:HB3	1:B:66:LYS:CG	2.35	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:Y:13:ILE:HD11	3:Y:30:ILE:HG23	1.85	0.56
2:C:943:MET:HE2	2:C:947:ASN:OD1	2.04	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)
2:D:713:ARG:HD3	4:D:13:HOH:O	2.05	0.56
2:C:830:LEU:O	2:C:830:LEU:HD23	2.04	0.56
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: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:HD22	2:C:856:ASN:N	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
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:7:HIS:O	1:A:10:LEU:HB3	2.07	0.55
2:D:813:GLU:HB3	2:D:814:LEU:CD1	2.37	0.55
1:B:54:ILE:HG12	1:B:67:VAL:HG22	1.88	0.55
1:A:5:ARG:NH2	1:A:61:PRO:HG3	2.21	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
2:C:638:LEU:HA	2:C:640:TYR:CE2	2.42	0.54
1:A:60:TYR:CG	1:A:61:PRO:HA	2.43	0.54
2:D:783:ASN:ND2	2:D:783:ASN:C	2.61	0.54
2:C:762:PHE:O	2:C:764:GLN:NE2	2.39	0.54
1:B:2:ALA:O	1:B:3:SER:C	2.45	0.54
1:A:50:PHE:CE1	1:A:73:ILE:HG13	2.43	0.54
3:Y:17:VAL:HG21	3:Y:56:LEU:CD1	2.38	0.54
2:C:761:ASN:ND2	2:C:761:ASN:O	2.40	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:CD2	2:C:711:PHE:N	2.76	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:C:653:LYS:HD2	2:C:890:MET:HG3	1.89	0.53
2:D:896:LEU:HD23	2:D:897:TYR:H	1.72	0.53
2:D:695:ARG:HD2	2:D:813:GLU:HG2	1.90	0.53
2:C:947:ASN:ND2	3:X:9:THR:OG1	2.41	0.53
2:C:637:GLY:O	2:C:640:TYR:CE2	2.60	0.53
1:B:113:PRO:O	1:B:115:PRO:HD3	2.09	0.53
1:B:55:HIS:HB3	1:B:66:LYS:CD	2.39	0.53
1:B:15:ARG:HD3	1:B:16:ASP:HB2	1.90	0.53
2:C:863:PHE:O	2:C:866:ALA:HB3	2.09	0.53
2:C:906:THR:CB	2:C:925:ARG:HG3	2.30	0.53
2:C:812:THR:CG2	2:C:817:ILE:HB	2.39	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:B:131:ARG:HG3	1:B:135:ASN:ND2	2.21	0.52
1:A:18:PRO:HB2	1:A:21:CYS:SG	2.50	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
3:X:9:THR:HG22	3:X:9:THR:O	2.09	0.52
1:B:9:GLU:OE1	1:B:99:ILE:N	2.39	0.52
1:A:11:ASN:O	1:A:15:ARG:HG3	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
2:C:761:ASN:HD22	2:C:761:ASN:N	2.08	0.52
1:A:25:PRO:HA	1:A:33:TRP:HA	1.91	0.52
3:Y:13:ILE:HG21	3:Y:34:GLU:OE2	2.09	0.52
3:X:26:VAL:O	3:X:30:ILE:HG13	2.10	0.52
2:C:815:LEU:N	2:C:815:LEU:HD12	2.25	0.52
2:C:757:ILE:HD13	2:C:794:TRP:CZ3	2.43	0.52
3:X:54:ARG:HG2	3:X:54:ARG:HH11	1.75	0.52
1:A:39:GLY:HA3	1:A:45:TYR:O	2.10	0.52
2:C:812:THR:HG21	2:C:817:ILE:HB	1.90	0.52
1:A:74:TYR:HB2	1:A:141:TRP:CD2	2.45	0.52
2:C:729:MET:CE	2:C:740:LEU:HD12	2.36	0.51
2:D:604:ARG:HG3	2:D:604:ARG:HH11	1.73	0.51
2:D:671:TYR:HE1	2:D:885:THR:HG21	1.73	0.51
1:B:9:GLU:OE1	1:B:99:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:863:PHE:O	2:C:867:VAL:HG23	2.10	0.51
3:X:67:LEU:H	3:X:67:LEU:HD12	1.75	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
2:D:596:ASN:O	2:D:597:ARG:HG2	2.10	0.51
2:C:590:LYS:HD2	2:C:625:LYS:O	2.10	0.51
2:C:765:THR:O	2:C:765:THR:HG23	2.10	0.51
1:B:142:THR:O	1:B:147:MET:HG3	2.09	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:O	2:D:845:GLN:HG2	2.10	0.51
3:X:63:LYS:O	3:X:64:GLU:HB2	2.09	0.51
2:C:812:THR:HA	2:C:815:LEU:O	2.10	0.51
1:B:11:ASN:ND2	1:B:11:ASN:N	2.56	0.51
1:B:101:LYS:O	1:B:105:SER:HB2	2.11	0.51
3:X:54:ARG:HG2	3:X:54:ARG:NH1	2.26	0.51
2:D:764:GLN:HG3	2:D:766:TYR:CE1	2.46	0.51
1:A:75:HIS:ND1	1:A:76:PRO:N	2.59	0.51
3:X:50:LEU:HD13	3:X:61:ILE:HD11	1.93	0.51
1:B:75:HIS:ND1	1:B:76:PRO:CD	2.73	0.51
2:D:729:MET:O	2:D:729:MET:HG2	2.11	0.51
2:C:583:TYR:CZ	2:C:587:LYS:HD2	2.46	0.51
2:C:910:TRP:HB3	2:C:927:ASP:HB3	1.92	0.50
1:B:60:TYR:CD1	1:B:61:PRO:HA	2.45	0.50
1:A:2:ALA:CB	2:C:758:ASP:OD2	2.59	0.50
1:B:144:LYS:NZ	1:B:144:LYS:HB2	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:D:814:LEU:C	2:D:815:LEU:HD12	2.32	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:C:578:LYS:O	2:C:582:ASP:OD1	2.29	0.50
3:X:23:ILE:HB	3:X:51:GLU:O	2.12	0.50
2:D:840:VAL:CG2	2:D:875:ARG:HD3	2.42	0.50
2:C:648:PHE:CE2	2:C:705:LYS:HG3	2.47	0.49
1:B:36:THR:HG22	1:B:51:PHE:HD2	1.77	0.49
2:D:671:TYR:CE1	2:D:885:THR:HG21	2.47	0.49
2:D:609:GLU:HB3	2:D:613:ARG:HH12	1.77	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:N	1:B:117:ASP:OD1	2.41	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
2:C:604:ARG:NH1	2:C:604:ARG:HB2	2.28	0.49
1:A:36:THR:CG2	2:D:868:LEU:CD1	2.90	0.49
3:Y:23:ILE:HB	3:Y:51:GLU:O	2.12	0.49
2:C:621:PRO:O	2:C:624:LEU:HD12	2.13	0.49
2:D:643:VAL:HG23	2:D:646:GLU:H	1.78	0.49
2:C:691:THR:HG22	2:C:806:ALA:O	2.12	0.49
1:A:74:TYR:HB2	1:A:141:TRP:CE3	2.48	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: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:582:ASP:O	2:D:586:LYS:HG3	2.13	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:N	2:D:746:ASN:ND2	2.61	0.48
2:D:618:VAL:HA	2:D:619:LYS:HE3	1.95	0.48
2:C:705:LYS:O	2:C:706:LEU:HD23	2.13	0.48
1:A:19:ALA:HB1	1:A:20:GLN:HE21	1.79	0.48
2:C:794:TRP:CD1	2:C:799:ARG:HD2	2.49	0.48
1:A:58:THR:HG21	2:C:760:GLU:CG	2.41	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
2:D:650:LEU:H	2:D:650:LEU:HD12	1.78	0.48
2:D:771:LYS:HE3	2:D:786:GLU:OE2	2.13	0.48
2:C:653:LYS:CD	2:C:890:MET:HG3	2.43	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
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
3:Y:13:ILE:O	3:Y:13:ILE:HG13	2.14	0.47
1:B:126:ILE:HG23	1:B:133:LYS:HG2	1.96	0.47
2:D:630:ILE:N	2:D:630:ILE:HD12	2.28	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:A:131:ARG:HG3	1:A:135:ASN:ND2	2.29	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:696:VAL:O	2:C:699:LEU:HB3	2.14	0.47
2:C:620:ARG:O	2:C:622:ASP:N	2.48	0.47
1:A:59:ASP:HB3	1:A:63:LYS:HG2	1.97	0.47
2:C:814:LEU:CB	2:C:815:LEU:HD12	2.45	0.47
3:Y:15:LEU:HD11	3:Y:30:ILE:HG12	1.96	0.47
2:D:869:LEU:HB3	2:D:938:ARG:HH12	1.80	0.47
1:B:13:LEU:CD2	1:B:18:PRO:HD2	2.44	0.47
1:A:64:PRO:HB3	1:A:93:TRP:CG	2.50	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:D:946:GLU:O	2:D:947:ASN:OD1	2.34	0.46
2:C:846:HIS:HA	2:D:638:LEU:HD12	1.98	0.46
2:C:726:LEU:HA	2:C:792:ILE:HD13	1.97	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
3:X:42:ARG:NH1	3:X:72:ARG:HE	2.14	0.46
2:D:909:GLN:CG	2:D:930:PRO:HG3	2.46	0.46
2:C:862:TRP:O	2:C:863:PHE:C	2.54	0.46
2:C:759:GLU:HB2	2:C:766:TYR:CE1	2.51	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: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
1:B:56:PHE:HE2	1:B:99:ILE:HD11	1.79	0.46
3:X:67:LEU:HD12	3:X:67:LEU:N	2.30	0.46
1:A:99:ILE:O	1:A:100:SER:C	2.54	0.46
2:C:949:GLN:HG2	2:C:949:GLN:O	2.16	0.46
1:A:8:LYS:HE2	2:C:752:ASP:HB2	1.98	0.46
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:891:ASN:HB2	2:D:895:GLU:HG3	1.97	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)
1:A:25:PRO:HB3	1:A:33:TRP:CD1	2.51	0.45
2:D:597:ARG:HH11	2:D:597:ARG:CB	2.28	0.45
2:C:599:GLU:O	2:C:614:ARG:NH1	2.49	0.45
2:D:691:THR:CG2	2:D:691:THR:O	2.64	0.45
3:X:37:PRO:HA	3:X:38:PRO:HD3	1.87	0.45
1:A:60:TYR:CE2	1:A:61:PRO:HB3	2.50	0.45
2:D:691:THR:HG22	2:D:691:THR:O	2.16	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
1:A:29:ASP:OD1	1:A:31:PHE:N	2.41	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
2:C:873:GLU:OE2	2:C:874:LYS:NZ	2.50	0.45
1:B:126:ILE:CG2	1:B:133:LYS:HG2	2.47	0.45
2:C:665:TYR:CE1	2:C:671:TYR:HA	2.52	0.45
1:A:72:ARG:HB2	1:A:145:TYR:CG	2.51	0.45
3:Y:59:TYR:O	3:Y:60:ASN:HB2	2.17	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
2:D:910:TRP:O	2:D:929:PRO:HA	2.16	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
1:B:69:PHE:O	1:B:82:GLY:HA3	2.17	0.45
2:C:910:TRP:O	2:C:929:PRO:HA	2.17	0.44
2:C:856:ASN:ND2	2:C:856:ASN:N	2.65	0.44
2:D:864:TRP:HA	2:D:864:TRP:CE3	2.52	0.44
2:C:657:ASN:ND2	2:C:890:MET:CE	2.80	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:D:604:ARG:NH1	2:D:604:ARG:HG3	2.30	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:C:828:LEU:O	2:C:828:LEU:HD12	2.17	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:D:602:LEU:O	2:D:602:LEU:HD12	2.17	0.44
3:X:42:ARG:HG3	3:X:72:ARG:CG	2.45	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)
1:A:63:LYS:HD3	2:C:736:TYR:HD2	1.82	0.44
2:C:699:LEU:HD12	2:C:703:HIS:HD2	1.83	0.44
2:D:931:TYR:CE1	2:D:940:LYS:HG2	2.53	0.44
2:D:854:CYS:HB2	2:D:855:PRO:CD	2.47	0.44
2:C:662:LEU:HA	2:C:662:LEU:HD23	1.81	0.44
1:A:22:SER:OG	1:A:36:THR:OG1	2.36	0.44
2:C:740:LEU:HD23	2:C:740:LEU:HA	1.82	0.44
1:A:62:PHE:HD1	2:C:736:TYR:CZ	2.35	0.44
2:C:759:GLU:HB2	2:C:766:TYR:CZ	2.53	0.44
3:Y:9:THR:O	3:Y:11:LYS:N	2.50	0.44
2:D:876:ILE:HG22	2:D:886:SER:HB2	1.99	0.44
2:D:754:MET:HA	2:D:777:ILE:O	2.18	0.44
3:Y:45:PHE:HB3	3:Y:50:LEU:HD21	1.99	0.43
2:D:591:PRO:HG2	2:D:594:ILE:HG21	1.99	0.43
2:C:710:PHE:CE1	2:C:833:CYS:O	2.71	0.43
2:C:652:SER:C	2:C:654:GLU:N	2.72	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:D:912:SER:C	2:D:914:GLU:H	2.21	0.43
2:C:895:GLU:OE1	2:D:631:GLU:OE2	2.37	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
3:Y:9:THR:C	3:Y:11:LYS:N	2.71	0.43
2:D:876:ILE:CG2	2:D:886:SER:HB2	2.49	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
3:Y:23:ILE:HG13	3:Y:50:LEU:HB3	2.01	0.43
2:D:949:GLN:OE1	2:D:949:GLN:N	2.40	0.43
3:X:11:LYS:CG	3:X:12:THR:N	2.81	0.43
2:C:630:ILE:HB	2:C:643:VAL:CG2	2.49	0.42
2:C:648:PHE:HE2	2:C:705:LYS:HG3	1.83	0.42
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:633:GLU:HA	2:C:636:LYS:HE3	2.01	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:891:ASN:HB2	2:C:895:GLU:HG3	2.02	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)
3:X:4:PHE:CE2	3:X:64:GLU:HG3	2.54	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
1:A:72:ARG:CG	1:A:72:ARG:HH11	2.30	0.42
2:D:840:VAL:HG12	2:D:840:VAL:O	2.19	0.42
2:D:912:SER:C	2:D:914:GLU:N	2.73	0.42
2:C:712:ILE:HA	4:C:3:HOH:O	2.19	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
2:C:608:PHE:CE1	2:C:655:MET:HG2	2.54	0.42
1:A:7:HIS:O	1:A:10:LEU:N	2.53	0.42
2:C:822:ILE:CG1	2:C:822:ILE:O	2.68	0.42
2:C:918:ARG:HH12	3:X:75:GLY:HA2	1.84	0.42
2:C:824:ASP:H	2:C:827:GLU:HB2	1.84	0.42
3:X:6:LYS:HB3	3:X:68:HIS:CD2	2.54	0.42
2:C:632:PHE:CE1	2:C:646:GLU:OE1	2.72	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
3:Y:72:ARG:HA	3:Y:72:ARG:HD3	1.40	0.42
2:D:823:PHE:HB3	2:D:827:GLU:HB2	2.00	0.42
2:C:848:ILE:CG1	2:C:906:THR:HG23	2.39	0.41
1:A:16:ASP:N	1:A:17:PRO:HD3	2.35	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
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:839:ASP:OD1	2:C:839:ASP:C	2.58	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
3:Y:42:ARG:NH2	3:Y:49:GLN:OE1	2.50	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
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: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:D:594:ILE:HD12	2:D:626:ALA:HB2	2.03	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:D:781:ASN:C	2:D:781:ASN:HD22	2.23	0.41
2:D:676:ASN:HD22	2:D:677:PRO:CD	2.33	0.41
2:C:762:PHE:N	2:C:762:PHE:CD1	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
3:Y:4:PHE:HB3	3:Y:12:THR:HG21	2.02	0.41
2:D:928:LEU:HD12	2:D:929:PRO:CD	2.50	0.41
2:C:794:TRP:CA	2:C:798:ASN:ND2	2.82	0.41
2:D:893:PHE:CD1	2:D:896:LEU:HD12	2.56	0.41
2:D:668:THR:HG22	2:D:897:TYR:CD2	2.56	0.41
2:D:635:GLU:HG3	2:D:635:GLU:H	1.45	0.41
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.85	0.41
2:C:938:ARG:HG2	2:C:942:LEU:HD12	2.02	0.41
2:D:577:PHE:CZ	2:D:830:LEU:HD23	2.55	0.40
2:C:585:ARG:O	2:C:588:LEU:HB2	2.22	0.40
2:D:835:LEU:HA	2:D:835:LEU:HD23	1.88	0.40
2:D:713:ARG:NH1	2:D:717:LYS:HD2	2.36	0.40
1:B:131:ARG:CG	1:B:135:ASN:HD21	2.25	0.40
3:X:31:GLN:HE21	3:X:37:PRO:HA	1.86	0.40
1:A:121:PRO:HG2	1:A:122:GLU:N	2.35	0.40
2:C:609:GLU:O	2:C:612:TYR:HB3	2.21	0.40
2:D:896:LEU:HD22	2:D:924:ASN:ND2	2.36	0.40
2:D:733:ASP:OD2	2:D:736:TYR:CB	2.54	0.40
2:C:659:TYR:HE2	2:D:627:ARG:HH21	1.68	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:D:814:LEU:N	2:D:814:LEU:CD1	2.82	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
2:D:622:ASP:C	2:D:624:LEU:H	2.25	0.40
2:D:906:THR:HB	2:D:925:ARG:HG3	2.04	0.40
1:B:79:ASN:ND2	1:B:83:SER:HB2	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/146 (99%)	130 (90%)	14 (10%)	0	100	100
1	B	144/146 (99%)	132 (92%)	11 (8%)	1 (1%)	26	65
2	C	374/385 (97%)	310 (83%)	61 (16%)	3 (1%)	24	63
2	D	372/385 (97%)	315 (85%)	56 (15%)	1 (0%)	46	80
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%)	39	75

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

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%)	27	64
1	B	130/130 (100%)	117 (90%)	13 (10%)	9	34
2	C	341/348 (98%)	315 (92%)	26 (8%)	16	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	340/348 (98%)	305 (90%)	35 (10%)	9	32
3	X	68/70 (97%)	64 (94%)	4 (6%)	24	60
3	Y	68/70 (97%)	63 (93%)	5 (7%)	17	51
All	All	1077/1096 (98%)	987 (92%)	90 (8%)	14	46

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

Some 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	146/146 (100%)	0.27	3 (2%) 67 44	74, 102, 110, 110	0
1	B	146/146 (100%)	0.30	2 (1%) 78 60	73, 98, 110, 110	0
2	C	376/385 (97%)	0.23	3 (0%) 87 75	64, 96, 110, 110	0
2	D	374/385 (97%)	0.14	0 100 100	63, 90, 110, 110	0
3	X	76/81 (93%)	1.90	31 (40%) 0 0	107, 110, 110, 110	0
3	Y	76/81 (93%)	1.64	27 (35%) 0 0	105, 110, 110, 110	0
All	All	1194/1224 (97%)	0.41	66 (5%) 29 12	63, 98, 110, 110	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	65	SER	6.3
3	X	66	THR	6.0
3	X	23	ILE	5.3
3	X	3	ILE	5.0
3	X	2	GLN	4.9
3	X	5	VAL	4.8
3	X	1	MET	4.7
3	X	13	ILE	4.5
3	X	12	THR	4.3
3	Y	1	MET	4.0
3	Y	15	LEU	4.0
3	Y	13	ILE	3.9
3	Y	67	LEU	3.6
3	Y	34	GLU	3.6
3	X	59	TYR	3.6
3	X	63	LYS	3.4
3	X	22	THR	3.4
3	X	64	GLU	3.3
1	A	30	MET	3.3

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Mol	Chain	Res	Type	RSRZ
3	Y	68	HIS	3.2
3	X	4	PHE	3.2
3	Y	35	GLY	3.1
3	X	21	ASP	3.1
3	X	61	ILE	3.1
3	X	9	THR	3.0
3	X	50	LEU	3.0
3	Y	2	GLN	3.0
3	Y	23	ILE	3.0
3	X	8	LEU	3.0
3	X	49	GLN	2.9
3	X	41	GLN	2.9
3	Y	21	ASP	2.9
3	Y	54	ARG	2.8
3	Y	64	GLU	2.8
3	X	45	PHE	2.8
3	Y	66	THR	2.8
3	X	30	ILE	2.8
3	Y	14	THR	2.7
3	Y	12	THR	2.7
3	Y	22	THR	2.7
3	Y	43	LEU	2.7
3	Y	17	VAL	2.6
3	Y	5	VAL	2.6
3	Y	59	TYR	2.6
3	Y	52	ASP	2.5
3	Y	36	ILE	2.5
3	X	51	GLU	2.5
1	A	18	PRO	2.4
1	B	21	CYS	2.4
3	Y	11	LYS	2.3
3	X	14	THR	2.3
3	X	44	ILE	2.3
1	A	130	ASP	2.3
3	X	67	LEU	2.3
2	C	583	TYR	2.2
3	Y	58	ASP	2.2
3	X	56	LEU	2.2
3	X	34	GLU	2.2
1	B	42	ASP	2.2
2	C	575	PHE	2.1
3	X	60	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	X	54	ARG	2.1
3	Y	44	ILE	2.1
3	Y	30	ILE	2.0
2	C	638	LEU	2.0
3	Y	10	GLY	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 carbohydrates 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.