



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 01:56 PM EDT

PDB ID : 2RF9  
Title : Crystal structure of the complex between the EGFR kinase domain and a Mig6 peptide  
Authors : Zhang, X.; Pickin, K.A.; Bose, R.; Jura, N.; Cole, P.A.; Kuriyan, J.  
Deposited on : unknown  
Resolution : 3.50 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

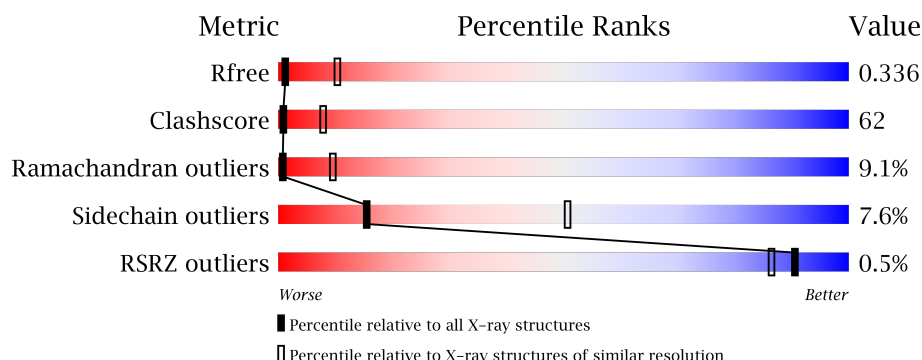
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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	330	<div> <div>25%</div> <div>48%</div> <div>11%</div> <div>15%</div> </div>
1	B	330	<div> <div>24%</div> <div>49%</div> <div>8%</div> <div>18%</div> </div>
2	C	65	<div> <div>25%</div> <div>15%</div> <div>58%</div> </div>
2	D	65	<div> <div>25%</div> <div>11%</div> <div>5%</div> <div>60%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4435 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2068	1336	345	372	15			
1	B	269	Total	C	N	O	S	0	0	0
			2010	1298	334	363	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	669	GLY	-	EXPRESSION TAG	UNP P00533
A	670	ALA	-	EXPRESSION TAG	UNP P00533
A	671	MET	-	EXPRESSION TAG	UNP P00533
B	669	GLY	-	EXPRESSION TAG	UNP P00533
B	670	ALA	-	EXPRESSION TAG	UNP P00533
B	671	MET	-	EXPRESSION TAG	UNP P00533

- Molecule 2 is a protein called ERBB receptor feedback inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	27	Total	C	N	O	S	0	0	0
			183	119	27	36	1			
2	D	26	Total	C	N	O	S	0	0	0
			174	113	26	34	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	310	GLY	-	EXPRESSION TAG	UNP Q9UJM3
C	311	PRO	-	EXPRESSION TAG	UNP Q9UJM3
C	312	LEU	-	EXPRESSION TAG	UNP Q9UJM3
C	313	GLY	-	EXPRESSION TAG	UNP Q9UJM3
C	314	SER	-	EXPRESSION TAG	UNP Q9UJM3
D	310	GLY	-	EXPRESSION TAG	UNP Q9UJM3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	311	PRO	-	EXPRESSION TAG	UNP Q9UJM3
D	312	LEU	-	EXPRESSION TAG	UNP Q9UJM3
D	313	GLY	-	EXPRESSION TAG	UNP Q9UJM3
D	314	SER	-	EXPRESSION TAG	UNP Q9UJM3

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

[illegible]

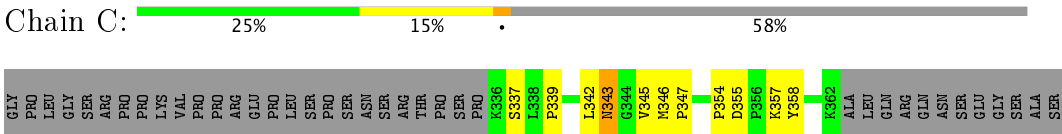
Chain B:

24% 49% 8% 18%

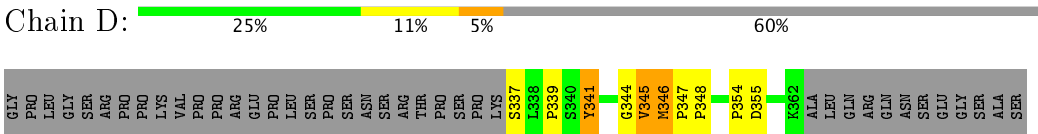
GLY ALA MET GLY GLU ALA ASN K677 A678 L679 L680 K684 K685 T686 P687 P688 K689 K690 K691 K692 K695 S696 G700 T701 W702 W703 W704 W705 W706 W707 W708 W709 E710 GLY GLU LYS VAL K715 L716 P717 W718 A719 T720 K721 E722 L723 W724 GLU ALA THR SER PRO LYS A731 W732 T733 E734 L735 W736 K737 E738 M741 W742 M743 V745 P748 H749 W750 W751 W752 T756 T757 L758 W759 T760 T761 W762 W763 L764 T765 T766 W767 L768 W769 T770 W771 T772 T773 T774 L775 L776 T777 T778 T779 E780 H781 P784 A785 T786 K787 K788 K789 K790 K791 K792 K793 K794 K795 K796 K797 K798 K799 K800 K801 K802 K803 K804 K805 K806 K807 K808 K809 K810 K811 K812 K813 K814 K815 K816 K817 K818 K819 K820 K821 K822 K823 K824 K825 K826 K827 K828 K829 K830 K831 K832 K833 K834 K835 K836 K837 K838 K839 K840 K841 K842 K843 K844 K845 K846 K847 K848 K849 K850 K851 K852 K853 K854 K855 K856 K857 K858 K859 K860 K861 K862 K863 K864 K865 K866 K867 K868 K869 K870 K871 K872 K873 K874 K875 K876 K877 K878 K879 K880 K881 K882 K883 K884 K885 K886 K887 K888 K889 K890 K891 K892 K893 K894 K895 K896 K897 K898 K899 K900 K901 K902 K903 K904 K905 K906 K907 K908 K909 K910 K911 K912 K913 K914 K915 K916 K917 K918 K919 K920 K921 K922 K923 K924 K925 K926 K927 K928 K929 K930 K931 K932 K933 K934 K935 K936 K937 K938 K939 K940 K941 K942 K943 K944 K945 K946 K947 K948 K949 K950 K951 K952 K953 K954 K955 K956 K957 K958 K959 K960 K961 K962 K963 K964 K965 K966 K967 K968 K969 K970 K971 K972 K973 K974 K975 K976 K977 K978 K979 K980 K981 K982 K983 K984 K985 K986 K987 K988 K989 K990 K991 K992 K993 K994 K995 K996 K997 K998 K999 K1000

ASP  
GLU  
TYR  
LEU  
ILE  
PRO  
GLN  
GLY

• Molecule 2: ERBB receptor feedback inhibitor 1



• Molecule 2: ERBB receptor feedback inhibitor 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	188.76 Å   42.65 Å   99.73 Å 90.00°   109.12°   90.00°	Depositor
Resolution (Å)	47.11 – 3.50 47.11 – 3.49	Depositor EDS
% Data completeness (in resolution range)	84.5 (47.11-3.50) 84.1 (47.11-3.49)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 3.48 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.272   ,   0.329 0.275   ,   0.336	Depositor DCC
$R_{free}$ test set	455 reflections (5.47%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.1	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33   ,   106.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4435	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.45% 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, 0.333 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	0.48	0/2114	0.74	1/2887 (0.0%)
1	B	0.46	0/2054	0.74	0/2800
2	C	0.65	0/190	0.77	0/264
2	D	0.57	0/181	0.83	0/251
All	All	0.48	0/4539	0.74	1/6202 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	729	PRO	N-CA-CB	5.40	109.78	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	891	TYR	Sidechain

### 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	2068	0	1961	258	0
1	B	2010	0	1902	249	0
2	C	183	0	152	18	0
2	D	174	0	138	27	0
All	All	4435	0	4153	532	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 62.

All (532) 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:341:TYR:CE2	2:D:347:PRO:HD2	1.80	1.17
2:D:341:TYR:HE2	2:D:347:PRO:HD2	0.95	1.09
2:D:339:PRO:CB	2:D:341:TYR:HE1	1.71	1.03
1:A:907:GLU:O	1:A:908:ARG:HD3	1.57	1.03
1:B:808:ARG:HH11	1:B:839:GLY:HA2	1.23	1.03
2:D:339:PRO:HB3	2:D:341:TYR:HE1	1.27	0.98
2:D:341:TYR:HE2	2:D:347:PRO:CD	1.78	0.96
1:A:859:LEU:HD13	1:A:903:LEU:HD23	1.47	0.95
1:B:696:SER:HB2	1:B:701:THR:HG22	1.49	0.93
1:A:739:ALA:HA	1:A:742:MET:HB3	1.50	0.93
2:D:339:PRO:HB2	2:D:341:TYR:CE1	2.04	0.93
1:A:864:HIS:O	1:A:866:ILE:HG13	1.68	0.92
2:D:341:TYR:CE2	2:D:347:PRO:CD	2.52	0.91
2:D:339:PRO:CB	2:D:341:TYR:CE1	2.54	0.91
1:A:775:LEU:HG	1:A:779:ARG:HE	1.36	0.89
1:A:812:ARG:HG3	1:A:867:TYR:CD2	2.08	0.89
1:B:781:HIS:O	1:B:785:ILE:HG13	1.75	0.86
1:B:696:SER:HA	1:B:701:THR:HA	1.58	0.86
1:B:902:ILE:HB	1:B:907:GLU:HG3	1.56	0.86
1:B:707:TRP:CE2	1:B:709:PRO:HG3	2.11	0.86
1:A:795:VAL:HG22	1:A:944:PHE:HB3	1.59	0.85
1:B:880:VAL:O	1:B:884:MET:HG2	1.75	0.85
1:B:696:SER:CB	1:B:701:THR:HG22	2.06	0.84
1:A:873:VAL:HG12	1:A:926:CYS:HB3	1.59	0.84
1:B:876:TYR:O	1:B:880:VAL:HG23	1.77	0.83
1:A:757:CYS:HB3	1:A:763:GLN:HB2	1.59	0.83
1:A:688:PHE:HA	1:A:706:LEU:O	1.79	0.83
1:B:815:ALA:O	1:B:819:VAL:HG23	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLU:O	1:A:707:TRP:HD1	1.63	0.82
1:B:777:TYR:OH	1:B:824:PRO:HG3	1.80	0.81
1:A:880:VAL:HB	1:A:923:MET:CE	2.11	0.80
1:B:881:TRP:N	1:B:923:MET:HE3	1.96	0.80
1:A:721:LYS:HZ1	1:A:830:THR:HG21	1.46	0.80
1:B:758:LEU:HD23	1:B:762:VAL:HG23	1.61	0.80
1:A:947:MET:HA	1:A:954:TYR:CE1	2.16	0.80
1:A:948:ALA:O	1:A:951:PRO:HD3	1.82	0.80
1:A:702:VAL:HG22	1:A:721:LYS:HA	1.61	0.80
1:A:830:THR:HG22	1:A:831:ASP:H	1.46	0.80
1:A:899:ILE:O	1:A:903:LEU:HB2	1.81	0.80
1:B:808:ARG:NH1	1:B:839:GLY:HA2	1.97	0.80
1:A:729:PRO:C	1:A:731:ALA:H	1.85	0.80
1:A:839:GLY:O	1:A:841:GLU:N	2.15	0.80
1:B:707:TRP:NE1	1:B:709:PRO:HG3	1.98	0.79
1:B:757:CYS:HB3	1:B:763:GLN:HB2	1.64	0.79
1:B:954:TYR:O	1:B:955:LEU:HD23	1.82	0.79
1:A:733:LYS:HE3	1:A:737:ASP:OD2	1.83	0.79
1:A:909:LEU:HD13	1:A:927:TRP:CH2	2.18	0.78
1:B:939:GLU:HA	1:B:942:ILE:HD12	1.65	0.78
1:B:769:MET:HG3	1:B:820:LEU:HD13	1.66	0.78
1:B:919:VAL:HG21	1:B:955:LEU:HD21	1.66	0.77
1:A:772:GLY:O	1:A:821:VAL:HG23	1.84	0.77
1:B:794:CYS:HA	1:B:797:ILE:HD12	1.65	0.76
1:A:721:LYS:NZ	1:A:830:THR:HG21	2.01	0.76
1:A:812:ARG:CZ	1:A:834:LEU:O	2.33	0.76
1:B:691:ILE:HB	1:B:704:LYS:O	1.86	0.75
1:A:911:GLN:NE2	2:C:339:PRO:HG3	2.02	0.75
1:B:702:VAL:CG2	1:B:721:LYS:HG2	2.16	0.75
1:A:753:LEU:HD11	1:A:764:LEU:HD22	1.68	0.75
1:A:702:VAL:HG13	1:A:720:ILE:O	1.87	0.74
1:B:775:LEU:HD11	1:B:779:ARG:HE	1.52	0.74
1:B:773:CYS:SG	1:B:775:LEU:HB3	2.28	0.74
1:B:793:TRP:O	1:B:797:ILE:HG13	1.85	0.74
1:A:760:SER:O	1:A:761:THR:HG23	1.87	0.74
1:B:930:ASP:O	1:B:933:SER:HB3	1.87	0.73
1:A:909:LEU:N	1:A:909:LEU:HD12	2.04	0.73
1:A:880:VAL:HB	1:A:923:MET:HE1	1.69	0.72
1:B:881:TRP:HB2	1:B:923:MET:HE1	1.71	0.72
1:B:795:VAL:HG12	1:B:799:LYS:HE3	1.71	0.72
1:A:753:LEU:HD12	1:A:766:THR:HG23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:PHE:HA	1:B:707:TRP:HA	1.70	0.72
1:B:947:MET:HA	1:B:954:TYR:CE1	2.25	0.72
1:A:696:SER:HB3	1:A:701:THR:HG23	1.70	0.72
1:A:830:THR:HG22	1:A:831:ASP:N	2.05	0.71
1:B:814:LEU:HD12	1:B:815:ALA:H	1.56	0.71
1:B:738:GLU:O	1:B:741:VAL:HG23	1.90	0.71
1:A:859:LEU:HD13	1:A:903:LEU:CD2	2.21	0.70
1:B:885:THR:HB	1:B:888:SER:HB2	1.71	0.70
1:B:899:ILE:O	1:B:903:LEU:HD13	1.91	0.70
1:A:795:VAL:O	1:A:799:LYS:HG3	1.92	0.70
1:A:876:TYR:O	1:A:880:VAL:HG23	1.91	0.70
1:B:957:ILE:N	1:B:957:ILE:HD12	2.07	0.70
1:A:696:SER:HA	1:A:701:THR:HA	1.73	0.70
1:A:722:GLU:O	1:A:722:GLU:HG2	1.92	0.70
1:A:787:SER:HA	1:A:955:LEU:HD12	1.74	0.70
2:D:339:PRO:HB3	2:D:341:TYR:CE1	2.20	0.69
1:A:916:THR:HG23	1:A:954:TYR:O	1.92	0.69
1:A:689:LYS:O	1:A:705:GLY:HA3	1.92	0.69
1:A:789:TYR:HA	1:A:792:ASN:HD22	1.58	0.69
1:B:771:PHE:HE2	1:B:823:THR:HA	1.56	0.69
1:B:741:VAL:HG11	1:B:809:LEU:HD21	1.74	0.69
1:A:775:LEU:CG	1:A:779:ARG:HE	2.06	0.68
1:A:721:LYS:O	1:A:763:GLN:HA	1.93	0.68
1:B:874:TRP:CE3	1:B:927:TRP:HA	2.29	0.68
1:A:789:TYR:O	1:A:792:ASN:HB2	1.94	0.68
1:B:869:HIS:O	1:B:872:ASP:HB2	1.93	0.68
1:B:909:LEU:HD12	1:B:909:LEU:H	1.59	0.68
1:B:814:LEU:HD23	1:B:876:TYR:HA	1.74	0.68
1:B:855:LYS:HE2	1:B:891:TYR:HB2	1.75	0.68
1:B:917:ILE:O	1:B:921:MET:HG2	1.93	0.68
1:A:785:ILE:HD13	1:A:793:TRP:HH2	1.59	0.67
1:A:809:LEU:CD1	1:A:810:VAL:H	2.08	0.67
1:A:729:PRO:O	1:A:731:ALA:N	2.28	0.67
1:A:770:PRO:HG2	1:A:771:PHE:H	1.60	0.67
1:B:684:LYS:C	1:B:686:THR:H	1.98	0.67
1:A:775:LEU:HG	1:A:779:ARG:NE	2.08	0.66
1:A:790:LEU:HD23	1:A:793:TRP:CZ3	2.29	0.66
1:B:809:LEU:HD22	1:B:837:LEU:HD13	1.77	0.66
1:B:710:GLU:O	1:B:710:GLU:HG2	1.95	0.66
1:B:762:VAL:HG22	1:B:763:GLN:N	2.11	0.66
1:A:687:GLU:O	1:A:707:TRP:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:GLU:HA	1:A:763:GLN:HG2	1.78	0.66
1:A:753:LEU:HD21	1:A:764:LEU:CD2	2.27	0.65
1:A:791:LEU:O	1:A:794:CYS:HB2	1.96	0.65
1:A:912:PRO:HB2	1:A:915:CYS:SG	2.37	0.65
1:B:911:GLN:HA	1:B:920:TYR:CE1	2.32	0.65
1:A:687:GLU:O	1:A:707:TRP:CD1	2.49	0.65
1:A:791:LEU:HD21	1:A:955:LEU:HD21	1.79	0.65
1:A:788:GLN:CD	1:A:792:ASN:HD21	2.00	0.65
1:A:792:ASN:O	1:A:793:TRP:C	2.34	0.65
1:A:881:TRP:N	1:A:923:MET:HE1	2.11	0.65
1:B:745:VAL:HA	1:B:803:TYR:OH	1.97	0.65
1:A:880:VAL:HB	1:A:923:MET:HE3	1.79	0.64
1:A:709:PRO:HB2	1:A:712:GLU:HB2	1.78	0.64
1:A:815:ALA:O	1:A:819:VAL:HG23	1.96	0.64
2:D:341:TYR:HD2	2:D:345:VAL:O	1.80	0.63
1:A:908:ARG:HB3	1:A:927:TRP:CE3	2.34	0.63
1:B:864:HIS:O	1:B:866:ILE:HG13	1.98	0.63
1:B:873:VAL:O	1:B:876:TYR:HB3	1.97	0.63
1:B:910:PRO:HG3	2:D:347:PRO:O	1.98	0.63
1:A:909:LEU:HD12	1:A:909:LEU:H	1.61	0.63
1:B:859:LEU:HG	1:B:863:LEU:HG	1.79	0.63
1:B:901:SER:HA	1:B:904:GLU:OE1	1.99	0.63
1:A:917:ILE:HG12	2:C:337:SER:HB2	1.79	0.63
1:B:930:ASP:HB3	1:B:933:SER:CB	2.28	0.63
1:A:788:GLN:HE21	1:A:788:GLN:HA	1.62	0.62
1:A:785:ILE:HD13	1:A:793:TRP:CH2	2.34	0.62
1:A:792:ASN:O	1:A:795:VAL:N	2.31	0.62
1:A:812:ARG:HG3	1:A:867:TYR:CE2	2.35	0.62
1:B:917:ILE:HG22	2:D:337:SER:HB2	1.81	0.62
1:A:917:ILE:HG12	2:C:337:SER:CB	2.30	0.62
1:A:712:GLU:O	1:A:714:VAL:N	2.33	0.62
1:A:881:TRP:HZ2	2:C:346:MET:HE3	1.63	0.62
1:B:788:GLN:HE21	1:B:792:ASN:HD21	1.48	0.61
1:B:876:TYR:CE2	1:B:940:LEU:HD13	2.35	0.61
1:A:734:GLU:O	1:A:735:ILE:C	2.37	0.61
1:A:799:LYS:O	1:A:802:ASN:HB3	2.00	0.61
1:A:732:ASN:HA	1:A:735:ILE:HG12	1.82	0.61
1:B:930:ASP:HB3	1:B:933:SER:HB2	1.83	0.61
1:A:854:ILE:HA	1:A:857:MET:SD	2.41	0.60
1:A:747:ASN:OD1	1:A:749:HIS:N	2.34	0.60
1:A:919:VAL:HG22	1:A:954:TYR:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:GLU:O	1:B:908:ARG:NH1	2.34	0.60
1:B:909:LEU:N	1:B:909:LEU:HD12	2.16	0.60
2:D:344:GLY:O	2:D:345:VAL:C	2.39	0.60
1:B:721:LYS:O	1:B:763:GLN:HA	2.01	0.60
1:B:925:LYS:O	1:B:928:MET:HG3	2.02	0.60
1:B:881:TRP:CA	1:B:923:MET:HE3	2.32	0.60
2:C:345:VAL:O	2:C:345:VAL:HG23	2.02	0.60
1:B:852:VAL:N	1:B:853:PRO:HD3	2.16	0.59
1:B:947:MET:HA	1:B:954:TYR:HE1	1.65	0.59
1:B:702:VAL:HG13	1:B:703:TYR:N	2.16	0.59
1:A:911:GLN:CD	2:C:339:PRO:HG3	2.22	0.59
1:B:796:GLN:O	1:B:799:LYS:HB2	2.03	0.59
1:A:805:GLU:HG3	1:A:869:HIS:ND1	2.18	0.59
1:B:758:LEU:CD2	1:B:762:VAL:HG23	2.30	0.59
1:B:909:LEU:HD13	1:B:927:TRP:CH2	2.37	0.59
1:A:770:PRO:HG2	1:A:771:PHE:CD1	2.38	0.59
2:C:355:ASP:OD1	2:C:357:LYS:N	2.29	0.59
1:A:753:LEU:HD21	1:A:764:LEU:HD22	1.83	0.59
1:A:937:PHE:O	1:A:938:ARG:C	2.40	0.59
1:B:870:GLN:HG3	1:B:931:ALA:O	2.02	0.59
1:B:917:ILE:CG2	2:D:337:SER:HB2	2.33	0.59
1:A:729:PRO:C	1:A:731:ALA:N	2.54	0.58
1:A:943:GLU:O	1:A:947:MET:HG3	2.02	0.58
1:A:730:LYS:C	1:A:732:ASN:H	2.04	0.58
1:A:876:TYR:HE2	1:A:940:LEU:HD22	1.68	0.58
1:B:912:PRO:HD2	1:B:915:CYS:HB2	1.85	0.58
1:B:745:VAL:CG2	1:B:752:ARG:HA	2.34	0.58
1:B:811:HIS:O	1:B:812:ARG:HB2	2.02	0.58
1:A:910:PRO:HB3	2:C:347:PRO:O	2.02	0.58
1:B:898:GLU:O	1:B:901:SER:N	2.37	0.58
1:B:917:ILE:HG13	1:B:917:ILE:O	2.04	0.58
1:A:881:TRP:CD2	1:A:909:LEU:HD23	2.39	0.58
1:B:837:LEU:HD12	1:B:838:LEU:H	1.69	0.58
1:B:805:GLU:HG3	1:B:869:HIS:ND1	2.19	0.58
1:B:700:GLY:O	1:B:701:THR:HG23	2.04	0.58
1:B:741:VAL:HG11	1:B:809:LEU:CD2	2.32	0.58
1:B:769:MET:HG3	1:B:820:LEU:CD1	2.33	0.58
1:B:946:LYS:O	1:B:949:ARG:N	2.36	0.58
1:A:723:LEU:H	1:A:723:LEU:HD23	1.69	0.57
1:B:937:PHE:O	1:B:941:ILE:HG13	2.04	0.57
1:B:764:LEU:O	1:B:765:ILE:HD13	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:LEU:CD1	1:A:909:LEU:H	2.17	0.57
1:A:809:LEU:HD13	1:A:810:VAL:H	1.70	0.57
1:B:766:THR:O	1:B:768:LEU:N	2.37	0.57
1:B:861:SER:HA	1:B:866:ILE:O	2.04	0.57
1:B:912:PRO:HB2	1:B:915:CYS:SG	2.45	0.57
1:B:707:TRP:O	1:B:709:PRO:HD3	2.05	0.57
1:A:921:MET:O	1:A:925:LYS:HB2	2.04	0.57
1:B:919:VAL:HG22	1:B:947:MET:SD	2.45	0.56
1:B:731:ALA:C	1:B:733:LYS:H	2.07	0.56
1:B:881:TRP:HB2	1:B:923:MET:CE	2.36	0.56
1:B:759:THR:OG1	1:B:760:SER:N	2.38	0.56
1:B:731:ALA:O	1:B:733:LYS:N	2.35	0.56
1:A:739:ALA:HB1	1:A:753:LEU:HD23	1.87	0.55
1:B:900:SER:O	1:B:904:GLU:HG3	2.06	0.55
1:A:845:TYR:HE2	1:A:847:ALA:HB2	1.72	0.55
1:A:712:GLU:C	1:A:714:VAL:H	2.08	0.55
1:B:870:GLN:HA	1:B:873:VAL:HG23	1.89	0.55
1:B:855:LYS:HZ3	1:B:889:LYS:HE2	1.70	0.55
1:A:700:GLY:HA3	1:A:723:LEU:HA	1.88	0.55
1:B:722:GLU:O	1:B:722:GLU:HG2	2.06	0.55
1:A:911:GLN:HA	1:A:920:TYR:CE1	2.42	0.54
1:A:874:TRP:HZ2	1:A:903:LEU:HD11	1.73	0.54
1:A:756:ILE:HD12	1:A:764:LEU:HD21	1.88	0.54
1:B:957:ILE:HG22	1:B:958:GLN:H	1.72	0.54
1:B:805:GLU:HG3	1:B:869:HIS:CE1	2.43	0.54
1:A:783:ASP:O	1:A:784:ASN:ND2	2.41	0.54
1:B:873:VAL:O	1:B:876:TYR:N	2.39	0.54
1:A:691:ILE:HG22	1:A:692:LYS:N	2.22	0.54
1:A:788:GLN:NE2	1:A:788:GLN:HA	2.23	0.54
1:B:799:LYS:HA	1:B:941:ILE:HD13	1.90	0.53
1:A:732:ASN:HA	1:A:735:ILE:CG1	2.39	0.53
1:A:914:ILE:O	1:A:955:LEU:HA	2.09	0.53
1:B:684:LYS:C	1:B:686:THR:N	2.62	0.53
1:A:750:VAL:O	1:A:752:ARG:N	2.41	0.53
1:A:898:GLU:O	1:A:902:ILE:HG12	2.08	0.53
1:A:788:GLN:HG3	1:A:789:TYR:N	2.23	0.53
1:A:858:ALA:HA	1:A:874:TRP:CD2	2.43	0.53
1:B:808:ARG:O	1:B:837:LEU:HD12	2.08	0.53
1:B:687:GLU:O	1:B:688:PHE:HB3	2.08	0.53
1:B:807:ARG:O	1:B:809:LEU:HD23	2.09	0.53
1:B:767:GLN:O	1:B:768:LEU:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:LEU:O	1:B:815:ALA:HB2	2.09	0.52
1:A:864:HIS:O	1:A:865:ARG:C	2.48	0.52
1:B:790:LEU:HA	1:B:793:TRP:CE3	2.44	0.52
1:B:937:PHE:CD2	1:B:940:LEU:HD12	2.43	0.52
1:A:777:TYR:OH	1:A:824:PRO:HG3	2.09	0.52
1:A:789:TYR:CA	1:A:792:ASN:HD22	2.21	0.52
1:A:908:ARG:HB3	1:A:927:TRP:HE3	1.74	0.52
1:B:732:ASN:O	1:B:736:LEU:HG	2.09	0.52
1:B:890:PRO:HB2	1:B:891:TYR:HD1	1.74	0.52
1:B:733:LYS:HA	1:B:736:LEU:HD12	1.91	0.52
1:B:790:LEU:HD23	1:B:793:TRP:CZ3	2.45	0.52
1:A:688:PHE:HD2	1:A:720:ILE:HD11	1.74	0.52
1:B:947:MET:HA	1:B:954:TYR:CD1	2.45	0.52
1:A:704:LYS:HA	1:A:719:ALA:HA	1.92	0.52
1:A:709:PRO:HD2	1:A:714:VAL:O	2.09	0.52
1:A:911:GLN:NE2	2:C:339:PRO:CG	2.73	0.52
1:B:794:CYS:HA	1:B:797:ILE:CD1	2.35	0.52
1:B:823:THR:OG1	1:B:824:PRO:HD2	2.09	0.52
1:B:748:PRO:O	1:B:828:LYS:HE2	2.09	0.51
1:A:941:ILE:O	1:A:945:SER:N	2.31	0.51
1:A:946:LYS:O	1:A:949:ARG:N	2.43	0.51
1:B:881:TRP:CE2	1:B:885:THR:HG21	2.45	0.51
1:B:898:GLU:O	1:B:899:ILE:C	2.49	0.51
1:B:891:TYR:O	1:B:894:ILE:HB	2.10	0.51
1:B:902:ILE:HB	1:B:907:GLU:CG	2.35	0.51
1:A:734:GLU:O	1:A:737:ASP:N	2.44	0.51
1:B:858:ALA:HA	1:B:874:TRP:CE2	2.45	0.51
1:A:909:LEU:HB2	1:A:927:TRP:HH2	1.75	0.51
1:B:702:VAL:HG22	1:B:721:LYS:HG2	1.91	0.51
1:B:938:ARG:O	1:B:942:ILE:HG13	2.11	0.51
1:B:947:MET:HG2	1:B:954:TYR:CE1	2.46	0.51
1:A:741:VAL:C	1:A:743:ALA:H	2.14	0.51
1:A:809:LEU:HD12	1:A:810:VAL:H	1.75	0.51
1:A:909:LEU:CD1	1:A:909:LEU:N	2.71	0.51
1:A:790:LEU:HA	1:A:793:TRP:CE3	2.46	0.51
1:A:947:MET:HA	1:A:954:TYR:HE1	1.72	0.51
2:C:342:LEU:O	2:C:343:ASN:CB	2.58	0.51
1:A:912:PRO:O	1:A:915:CYS:HB2	2.10	0.51
1:A:916:THR:C	1:A:918:ASP:H	2.14	0.51
1:A:823:THR:HG23	1:A:826:HIS:N	2.26	0.51
1:A:890:PRO:O	1:A:891:TYR:HD1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:LEU:O	1:B:836:LYS:HE3	2.11	0.51
1:A:730:LYS:C	1:A:732:ASN:N	2.62	0.50
1:B:815:ALA:HA	1:B:879:THR:HG23	1.93	0.50
1:A:768:LEU:HD12	1:A:769:MET:H	1.77	0.50
1:A:790:LEU:HD23	1:A:793:TRP:HZ3	1.73	0.50
1:A:938:ARG:O	1:A:941:ILE:HG13	2.11	0.50
1:B:795:VAL:O	1:B:799:LYS:HG3	2.11	0.50
1:A:709:PRO:O	1:A:710:GLU:C	2.49	0.50
1:A:739:ALA:HA	1:A:742:MET:CB	2.33	0.50
1:B:798:ALA:O	1:B:802:ASN:N	2.43	0.50
1:A:790:LEU:CD2	1:A:793:TRP:HZ3	2.25	0.50
1:B:793:TRP:CD1	1:B:827:VAL:HG21	2.46	0.50
1:A:917:ILE:HG12	2:C:337:SER:OG	2.11	0.50
1:B:890:PRO:HB2	1:B:891:TYR:CD1	2.46	0.50
1:A:711:GLY:O	1:A:712:GLU:C	2.49	0.50
1:B:812:ARG:HH21	1:B:836:LYS:HE3	1.77	0.50
1:B:719:ALA:O	1:B:765:ILE:HA	2.12	0.50
1:B:912:PRO:HG2	1:B:915:CYS:SG	2.52	0.50
1:B:921:MET:O	1:B:925:LYS:HE3	2.12	0.50
1:B:858:ALA:HA	1:B:874:TRP:CD2	2.47	0.50
1:B:876:TYR:HA	1:B:879:THR:OG1	2.12	0.50
1:B:894:ILE:HD11	2:D:348:PRO:HB3	1.94	0.50
1:A:880:VAL:CB	1:A:923:MET:HE1	2.42	0.49
1:B:858:ALA:HB1	1:B:860:GLU:OE1	2.12	0.49
1:A:775:LEU:HD21	1:A:779:ARG:HH21	1.76	0.49
1:B:820:LEU:O	1:B:827:VAL:HG12	2.12	0.49
1:B:912:PRO:HD2	1:B:915:CYS:CB	2.41	0.49
1:B:917:ILE:HG22	2:D:337:SER:CB	2.42	0.49
1:A:753:LEU:HA	1:A:766:THR:CG2	2.43	0.49
1:A:753:LEU:HA	1:A:766:THR:HG22	1.93	0.49
1:A:934:ARG:HB3	1:A:935:PRO:CD	2.43	0.49
1:A:787:SER:OG	1:A:951:PRO:HB2	2.13	0.49
1:B:793:TRP:HD1	1:B:827:VAL:CG2	2.25	0.49
1:B:735:ILE:HD12	1:B:833:GLY:CA	2.42	0.49
1:A:845:TYR:HB3	1:A:867:TYR:HB2	1.95	0.49
1:A:879:THR:O	1:A:883:LEU:HG	2.12	0.49
1:B:793:TRP:O	1:B:796:GLN:HB2	2.12	0.49
1:B:958:GLN:O	1:B:959:GLY:O	2.30	0.49
1:A:781:HIS:HB3	1:A:784:ASN:HB2	1.95	0.49
1:B:902:ILE:O	1:B:907:GLU:HB2	2.13	0.49
1:B:821:VAL:HA	1:B:827:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:THR:CB	1:B:888:SER:HB2	2.43	0.49
1:A:909:LEU:HB2	1:A:927:TRP:CH2	2.48	0.49
1:B:677:GLN:O	1:B:678:ALA:HB2	2.13	0.49
1:B:919:VAL:HG21	1:B:955:LEU:CD2	2.40	0.49
1:A:683:LEU:HD11	1:A:765:ILE:HG13	1.95	0.48
1:B:814:LEU:HD23	1:B:876:TYR:CA	2.43	0.48
1:A:741:VAL:O	1:A:744:SER:N	2.45	0.48
1:A:890:PRO:C	1:A:891:TYR:CD1	2.87	0.48
1:B:748:PRO:HB2	1:B:826:HIS:NE2	2.29	0.48
1:B:846:HIS:HA	1:B:865:ARG:O	2.13	0.48
1:A:874:TRP:CZ2	1:A:903:LEU:HD21	2.48	0.48
1:B:835:ALA:O	1:B:836:LYS:HD3	2.13	0.48
1:A:790:LEU:HD23	1:A:793:TRP:CE3	2.49	0.48
1:A:830:THR:CG2	1:A:831:ASP:H	2.18	0.48
1:A:854:ILE:O	1:A:857:MET:HG3	2.13	0.48
1:A:775:LEU:CD2	1:A:779:ARG:HE	2.26	0.48
1:B:794:CYS:SG	1:B:880:VAL:HG13	2.53	0.48
1:B:939:GLU:O	1:B:942:ILE:N	2.47	0.48
1:A:762:VAL:C	1:A:763:GLN:HG3	2.34	0.48
1:B:691:ILE:HG13	1:B:705:GLY:HA2	1.96	0.48
1:B:762:VAL:HG22	1:B:763:GLN:H	1.75	0.48
1:B:868:THR:H	1:B:871:SER:CB	2.26	0.48
1:B:685:GLU:HA	1:B:688:PHE:CZ	2.48	0.48
1:A:792:ASN:O	1:A:794:CYS:N	2.47	0.48
1:A:874:TRP:C	1:A:874:TRP:CD1	2.87	0.48
1:B:930:ASP:CB	1:B:933:SER:HB2	2.44	0.48
1:A:912:PRO:HD3	1:A:920:TYR:CD1	2.49	0.48
1:B:775:LEU:CD1	1:B:779:ARG:HE	2.23	0.47
1:B:741:VAL:CG1	1:B:809:LEU:HD21	2.43	0.47
1:A:751:CYS:O	1:A:752:ARG:C	2.53	0.47
1:A:898:GLU:HA	1:A:901:SER:OG	2.14	0.47
1:B:695:GLY:O	1:B:702:VAL:N	2.47	0.47
1:B:868:THR:H	1:B:871:SER:HB3	1.79	0.47
1:A:688:PHE:HD2	1:A:720:ILE:CD1	2.27	0.47
1:A:795:VAL:HG12	1:A:799:LYS:HE3	1.96	0.47
1:A:823:THR:CG2	1:A:826:HIS:HB2	2.45	0.47
1:B:813:ASP:O	1:B:813:ASP:CG	2.51	0.47
2:D:341:TYR:N	2:D:341:TYR:CD1	2.82	0.47
1:A:810:VAL:O	1:A:835:ALA:HA	2.14	0.47
1:A:753:LEU:HD21	1:A:764:LEU:HD21	1.97	0.47
1:B:879:THR:O	1:B:883:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:909:LEU:HD13	1:B:927:TRP:CZ3	2.50	0.47
1:A:752:ARG:O	1:A:766:THR:HG22	2.14	0.47
1:B:762:VAL:CG2	1:B:763:GLN:N	2.77	0.47
1:B:735:ILE:HD12	1:B:833:GLY:HA2	1.95	0.47
1:B:947:MET:HG2	1:B:954:TYR:CD1	2.49	0.47
1:B:870:GLN:HA	1:B:873:VAL:CG2	2.45	0.47
1:A:708:ILE:O	1:A:710:GLU:N	2.48	0.46
2:D:341:TYR:CD2	2:D:347:PRO:CD	2.97	0.46
1:A:776:ASP:O	1:A:779:ARG:HB2	2.15	0.46
1:B:814:LEU:HD23	1:B:876:TYR:HB2	1.96	0.46
1:B:799:LYS:HA	1:B:941:ILE:CD1	2.45	0.46
1:B:957:ILE:CD1	1:B:957:ILE:N	2.76	0.46
1:B:745:VAL:O	1:B:745:VAL:HG23	2.16	0.46
1:A:811:HIS:O	1:A:812:ARG:HB3	2.15	0.46
1:A:718:VAL:HG21	1:A:765:ILE:HG23	1.98	0.46
1:A:707:TRP:CE3	1:A:716:ILE:HD12	2.51	0.46
1:A:721:LYS:NZ	1:A:830:THR:CG2	2.75	0.46
1:B:823:THR:HG22	1:B:826:HIS:HB3	1.96	0.46
1:B:742:MET:HA	1:B:745:VAL:HG13	1.97	0.46
1:B:891:TYR:OH	1:B:909:LEU:HD11	2.16	0.46
1:A:811:HIS:CE1	1:A:813:ASP:O	2.69	0.46
1:B:864:HIS:HB2	1:B:866:ILE:CD1	2.46	0.46
1:A:809:LEU:CD1	1:A:835:ALA:HB1	2.46	0.46
1:B:796:GLN:O	1:B:799:LYS:N	2.48	0.45
1:B:864:HIS:HB2	1:B:866:ILE:HD12	1.96	0.45
1:B:794:CYS:O	1:B:795:VAL:C	2.53	0.45
1:B:889:LYS:HG2	1:B:890:PRO:N	2.31	0.45
1:B:764:LEU:HD23	1:B:764:LEU:HA	1.74	0.45
1:B:793:TRP:HD1	1:B:827:VAL:HG21	1.81	0.45
1:A:734:GLU:O	1:A:738:GLU:N	2.35	0.45
1:A:778:VAL:HG12	1:A:785:ILE:CD1	2.45	0.45
1:A:907:GLU:C	1:A:908:ARG:HD3	2.33	0.45
1:B:745:VAL:HG21	1:B:752:ARG:HA	1.97	0.45
1:B:749:HIS:HA	1:B:828:LYS:HG2	1.97	0.45
1:B:803:TYR:O	1:B:806:ASP:HB2	2.16	0.45
1:B:830:THR:HG22	1:B:831:ASP:O	2.16	0.45
1:B:854:ILE:C	1:B:856:TRP:H	2.20	0.45
1:B:925:LYS:HE3	1:B:925:LYS:HB2	1.61	0.45
1:B:930:ASP:CG	1:B:933:SER:HB2	2.37	0.45
1:A:712:GLU:C	1:A:714:VAL:N	2.69	0.45
1:A:831:ASP:CG	1:A:833:GLY:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:803:TYR:HA	1:B:806:ASP:HB2	1.98	0.45
1:A:874:TRP:O	1:A:874:TRP:CD1	2.70	0.45
1:A:814:LEU:HD12	1:A:815:ALA:N	2.32	0.45
1:A:823:THR:C	1:A:825:GLN:N	2.68	0.45
1:B:687:GLU:O	1:B:688:PHE:CB	2.64	0.45
1:A:768:LEU:HD12	1:A:769:MET:N	2.32	0.45
1:B:719:ALA:O	1:B:765:ILE:HD13	2.17	0.45
1:A:917:ILE:CG1	2:C:337:SER:HB2	2.47	0.45
1:A:911:GLN:HE21	2:C:339:PRO:HD3	1.82	0.45
1:A:708:ILE:HG23	1:A:708:ILE:O	2.17	0.44
1:A:940:LEU:O	1:A:944:PHE:HD2	2.00	0.44
1:A:787:SER:N	1:A:957:ILE:CD1	2.81	0.44
1:B:884:MET:HE1	1:B:919:VAL:HG11	1.99	0.44
1:A:743:ALA:C	1:A:745:VAL:H	2.21	0.44
1:A:830:THR:CG2	1:A:831:ASP:N	2.75	0.44
1:A:876:TYR:CE2	1:A:940:LEU:HD13	2.52	0.44
1:B:939:GLU:O	1:B:940:LEU:C	2.55	0.44
1:A:924:VAL:O	2:C:358:TYR:HE2	1.99	0.44
1:B:690:LYS:HE3	1:B:690:LYS:O	2.18	0.44
1:B:798:ALA:HA	1:B:801:MET:HB2	1.98	0.44
1:B:891:TYR:O	1:B:892:ASP:C	2.56	0.44
1:A:774:LEU:HD12	1:A:774:LEU:O	2.18	0.44
1:B:748:PRO:HB2	1:B:826:HIS:CE1	2.53	0.44
2:D:341:TYR:CD2	2:D:347:PRO:HD3	2.52	0.44
1:A:696:SER:CB	1:A:701:THR:HG23	2.43	0.44
1:A:946:LYS:O	1:A:947:MET:C	2.54	0.44
1:B:880:VAL:HA	1:B:883:LEU:CD1	2.48	0.44
1:B:913:PRO:HD3	2:D:346:MET:SD	2.57	0.44
1:A:684:LYS:O	1:A:686:THR:N	2.42	0.44
1:A:741:VAL:C	1:A:743:ALA:N	2.70	0.44
1:B:700:GLY:O	1:B:701:THR:CG2	2.66	0.44
1:B:821:VAL:HG13	1:B:827:VAL:HG13	2.00	0.44
1:B:891:TYR:O	1:B:892:ASP:O	2.36	0.44
1:A:753:LEU:CD1	1:A:764:LEU:HD22	2.43	0.44
1:A:891:TYR:O	1:A:892:ASP:C	2.56	0.44
1:B:881:TRP:CZ2	1:B:885:THR:HG21	2.53	0.44
1:B:891:TYR:CZ	1:B:909:LEU:HG	2.53	0.44
1:B:770:PRO:HG2	1:B:771:PHE:H	1.82	0.43
1:B:873:VAL:O	1:B:874:TRP:C	2.55	0.43
1:A:741:VAL:O	1:A:743:ALA:N	2.51	0.43
1:A:855:LYS:HG2	1:A:899:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:TRP:CZ3	1:B:927:TRP:HA	2.53	0.43
1:A:787:SER:O	1:A:788:GLN:C	2.56	0.43
1:A:852:VAL:O	1:A:853:PRO:C	2.57	0.43
1:A:756:ILE:HG13	1:A:763:GLN:O	2.19	0.43
1:A:775:LEU:O	1:A:779:ARG:HD2	2.17	0.43
1:B:796:GLN:OE1	1:B:827:VAL:HG23	2.18	0.43
1:B:872:ASP:O	1:B:873:VAL:C	2.57	0.43
1:A:685:GLU:O	1:A:686:THR:HG23	2.18	0.43
1:A:711:GLY:O	1:A:713:LYS:N	2.51	0.43
1:A:811:HIS:O	1:A:812:ARG:CB	2.66	0.43
1:A:880:VAL:O	1:A:881:TRP:C	2.56	0.43
1:B:912:PRO:HA	1:B:913:PRO:HD3	1.90	0.43
1:A:707:TRP:O	1:A:709:PRO:HD3	2.19	0.43
1:A:716:ILE:HA	1:A:717:PRO:HD3	1.66	0.43
1:B:935:PRO:HA	1:B:939:GLU:OE1	2.19	0.43
1:A:707:TRP:N	1:A:716:ILE:O	2.49	0.43
1:B:959:GLY:C	1:B:961:GLU:H	2.21	0.43
1:A:788:GLN:CA	1:A:788:GLN:NE2	2.80	0.43
1:A:773:CYS:HA	1:A:819:VAL:O	2.19	0.43
1:B:854:ILE:C	1:B:856:TRP:N	2.72	0.43
1:B:924:VAL:O	1:B:927:TRP:N	2.40	0.43
1:A:940:LEU:O	1:A:944:PHE:HB2	2.18	0.42
1:B:810:VAL:HG12	1:B:810:VAL:O	2.18	0.42
1:B:903:LEU:HG	1:B:908:ARG:HH12	1.85	0.42
1:A:748:PRO:HB2	1:A:826:HIS:NE2	2.34	0.42
1:A:759:THR:C	1:A:761:THR:H	2.23	0.42
1:A:787:SER:CB	1:A:951:PRO:HB2	2.49	0.42
1:A:944:PHE:C	1:A:946:LYS:H	2.22	0.42
1:B:691:ILE:HG22	1:B:692:LYS:N	2.34	0.42
1:B:911:GLN:HA	1:B:920:TYR:CD1	2.54	0.42
1:B:951:PRO:HG2	1:B:952:GLN:H	1.84	0.42
2:D:339:PRO:HB2	2:D:341:TYR:CD1	2.51	0.42
1:A:777:TYR:CE1	1:A:781:HIS:CD2	3.08	0.42
1:A:791:LEU:O	1:A:795:VAL:HG23	2.19	0.42
1:A:906:GLY:HA2	1:A:908:ARG:NH1	2.34	0.42
1:A:722:GLU:CA	1:A:763:GLN:HG2	2.47	0.42
1:A:813:ASP:HB2	1:A:852:VAL:HG22	2.02	0.42
1:A:876:TYR:CD2	1:A:940:LEU:HD13	2.54	0.42
1:A:953:ARG:HG2	1:A:953:ARG:O	2.19	0.42
1:A:764:LEU:HA	1:A:764:LEU:HD23	1.88	0.42
1:B:702:VAL:CG1	1:B:703:TYR:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:881:TRP:CZ3	1:B:888:SER:O	2.73	0.42
2:C:354:PRO:HB2	2:D:339:PRO:HA	2.02	0.42
1:A:777:TYR:CD1	1:A:781:HIS:CD2	3.07	0.42
1:A:788:GLN:O	1:A:792:ASN:ND2	2.52	0.42
1:A:890:PRO:O	1:A:891:TYR:CD1	2.71	0.42
1:B:770:PRO:HG2	1:B:771:PHE:N	2.34	0.42
1:B:788:GLN:HE21	1:B:792:ASN:ND2	2.14	0.42
1:A:823:THR:C	1:A:825:GLN:H	2.22	0.41
1:A:819:VAL:CG1	1:A:828:LYS:O	2.68	0.41
1:A:874:TRP:HD1	1:A:874:TRP:O	2.03	0.41
1:B:916:THR:HG23	1:B:954:TYR:O	2.19	0.41
2:D:354:PRO:O	2:D:355:ASP:C	2.56	0.41
1:A:819:VAL:HG12	1:A:828:LYS:O	2.19	0.41
1:B:731:ALA:C	1:B:733:LYS:N	2.73	0.41
1:B:870:GLN:O	1:B:873:VAL:HB	2.20	0.41
1:B:880:VAL:HG12	1:B:884:MET:CE	2.50	0.41
1:A:785:ILE:HG21	1:A:790:LEU:HG	2.03	0.41
1:B:914:ILE:O	1:B:914:ILE:HG13	2.20	0.41
1:B:912:PRO:CG	1:B:915:CYS:SG	3.09	0.41
1:A:859:LEU:HD12	1:A:859:LEU:HA	1.71	0.41
1:A:876:TYR:CE1	1:A:880:VAL:CG2	3.04	0.41
1:A:878:VAL:O	1:A:881:TRP:HB3	2.19	0.41
1:A:920:TYR:CE2	1:A:924:VAL:HG21	2.56	0.41
1:B:690:LYS:O	1:B:690:LYS:HD2	2.21	0.41
1:B:748:PRO:O	1:B:828:LYS:HG2	2.21	0.41
1:A:885:THR:HB	1:A:888:SER:OG	2.21	0.41
1:A:877:GLY:O	1:A:923:MET:CE	2.69	0.41
1:B:815:ALA:CA	1:B:879:THR:HG23	2.50	0.41
1:A:770:PRO:CG	1:A:771:PHE:H	2.31	0.41
2:D:341:TYR:CE2	2:D:347:PRO:HD3	2.52	0.41
2:D:341:TYR:CD2	2:D:345:VAL:O	2.68	0.41
2:D:346:MET:HA	2:D:347:PRO:HD2	1.81	0.41
1:A:904:GLU:C	1:A:906:GLY:H	2.25	0.41
1:A:957:ILE:HG13	1:A:957:ILE:H	1.77	0.41
1:A:788:GLN:CG	1:A:789:TYR:N	2.83	0.41
1:A:917:ILE:HG23	2:C:337:SER:O	2.21	0.41
1:B:784:ASN:HD22	1:B:784:ASN:HA	1.55	0.41
1:B:909:LEU:CD1	1:B:909:LEU:H	2.32	0.41
1:A:796:GLN:HA	1:A:799:LYS:HD2	2.04	0.40
1:A:916:THR:HA	2:C:337:SER:O	2.21	0.40
1:B:756:ILE:HG23	1:B:756:ILE:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:TYR:N	2:D:341:TYR:HD1	2.18	0.40
1:A:890:PRO:O	1:A:891:TYR:HB2	2.22	0.40
1:B:742:MET:HA	1:B:745:VAL:CG1	2.51	0.40
1:B:771:PHE:HD2	1:B:821:VAL:O	2.04	0.40
1:B:774:LEU:O	1:B:777:TYR:HB3	2.21	0.40
1:B:790:LEU:HD23	1:B:793:TRP:HZ3	1.86	0.40
1:A:850:GLY:O	1:A:851:LYS:HB3	2.22	0.40
1:B:793:TRP:CD1	1:B:827:VAL:CG2	3.02	0.40
1:B:855:LYS:NZ	1:B:889:LYS:HE2	2.35	0.40
2:C:346:MET:HA	2:C:347:PRO:HD2	1.96	0.40
1:A:762:VAL:HG22	1:A:763:GLN:N	2.37	0.40
1:A:777:TYR:C	1:A:779:ARG:H	2.24	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	274/330 (83%)	188 (69%)	57 (21%)	29 (11%)	0	7
1	B	259/330 (78%)	183 (71%)	54 (21%)	22 (8%)	1	11
2	C	25/65 (38%)	21 (84%)	3 (12%)	1 (4%)	3	30
2	D	24/65 (37%)	15 (62%)	8 (33%)	1 (4%)	3	28
All	All	582/790 (74%)	407 (70%)	122 (21%)	53 (9%)	1	9

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	713	LYS
1	A	730	LYS
1	A	751	CYS

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Mol	Chain	Res	Type
1	A	788	GLN
1	A	835	ALA
1	A	840	ALA
1	A	851	LYS
1	B	678	ALA
1	B	679	LEU
1	B	767	GLN
1	B	892	ASP
1	B	959	GLY
2	C	343	ASN
2	D	345	VAL
1	A	685	GLU
1	A	712	GLU
1	A	767	GLN
1	A	770	PRO
1	A	836	LYS
1	A	895	PRO
1	B	691	ILE
1	B	732	ASN
1	B	873	VAL
1	A	710	GLU
1	A	735	ILE
1	A	792	ASN
1	A	808	ARG
1	A	852	VAL
1	A	858	ALA
1	A	892	ASP
1	B	688	PHE
1	B	768	LEU
1	B	815	ALA
1	B	855	LYS
1	A	679	LEU
1	A	742	MET
1	A	744	SER
1	A	793	TRP
1	B	687	GLU
1	B	770	PRO
1	A	676	ASN
1	A	709	PRO
1	A	855	LYS
1	B	680	LEU
1	B	685	GLU

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Mol	Chain	Res	Type
1	B	885	THR
1	B	951	PRO
1	B	960	ASP
1	B	717	PRO
1	B	797	ILE
1	B	913	PRO
1	A	917	ILE
1	A	691	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	203/288 (70%)	188 (93%)	15 (7%)	16	52
1	B	200/288 (69%)	184 (92%)	16 (8%)	14	48
2	C	18/58 (31%)	18 (100%)	0	100	100
2	D	16/58 (28%)	14 (88%)	2 (12%)	5	26
All	All	437/692 (63%)	404 (92%)	33 (8%)	15	51

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	745	VAL
1	A	761	THR
1	A	766	THR
1	A	809	LEU
1	A	814	LEU
1	A	823	THR
1	A	827	VAL
1	A	834	LEU
1	A	857	MET
1	A	865	ARG
1	A	895	PRO
1	A	901	SER
1	A	913	PRO

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Mol	Chain	Res	Type
1	A	918	ASP
1	A	957	ILE
1	B	690	LYS
1	B	702	VAL
1	B	707	TRP
1	B	723	LEU
1	B	734	GLU
1	B	741	VAL
1	B	751	CYS
1	B	784	ASN
1	B	827	VAL
1	B	862	ILE
1	B	875	SER
1	B	879	THR
1	B	909	LEU
1	B	914	ILE
1	B	932	ASP
1	B	957	ILE
2	D	341	TYR
2	D	346	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	788	GLN
1	A	792	ASN
1	A	911	GLN
1	B	749	HIS
1	B	781	HIS
1	B	784	ASN
1	B	788	GLN
1	B	802	ASN
1	B	811	HIS
1	B	911	GLN

### 5.3.3 RNA ⓘ

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	280/330 (84%)	-0.38	1 (0%) 92 89	24, 62, 106, 126	0
1	B	269/330 (81%)	-0.28	2 (0%) 87 82	41, 71, 102, 111	0
2	C	27/65 (41%)	0.00	0 100 100	71, 84, 98, 100	0
2	D	26/65 (40%)	-0.37	0 100 100	68, 83, 92, 102	0
All	All	602/790 (76%)	-0.32	3 (0%) 90 86	24, 70, 102, 126	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	953	ARG	2.2
1	B	952	GLN	2.2
1	A	676	ASN	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.