Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:44 am BST

PDB ID	:	2Z6E
Title	:	Crystal Structure of Human DAAM1 FH2
Authors	:	Yamashita, M.; Higashi, T.; Sato, Y.; Shirakawa, R.; Kita, T.; Horiuchi, H.; Fukai, S.; Nureki, O.
Deposited on	:	2007-07-31
Resolution	:	2.80 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 ①) were used in the production of this report:

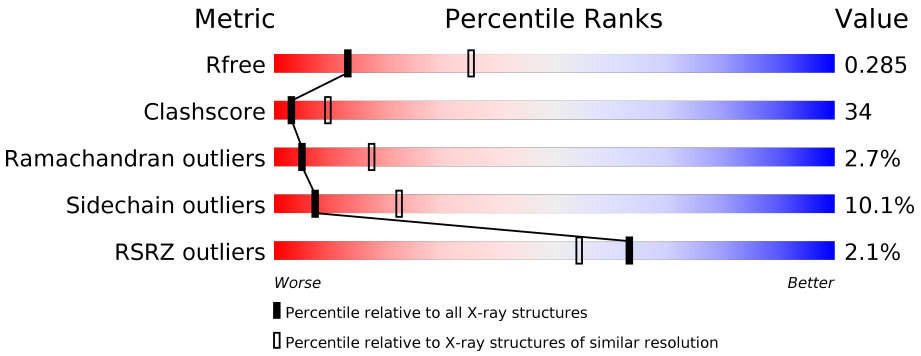
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	419	% 42% 44% 6% 7%
1	B	419	% 45% 40% 8% 5%
1	C	419	5% 39% 45% 6% 10%
1	D	419	% 42% 44% 7% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12750 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 Disheveled-associated activator of morphogenesis 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3156	1998	540	609	9			
1	B	396	Total	C	N	O	S	0	0	0
			3219	2042	550	617	10			
1	C	379	Total	C	N	O	S	0	0	0
			3080	1951	524	597	8			
1	D	390	Total	C	N	O	S	0	0	0
			3173	2007	543	614	9			

- Molecule 2 is water.

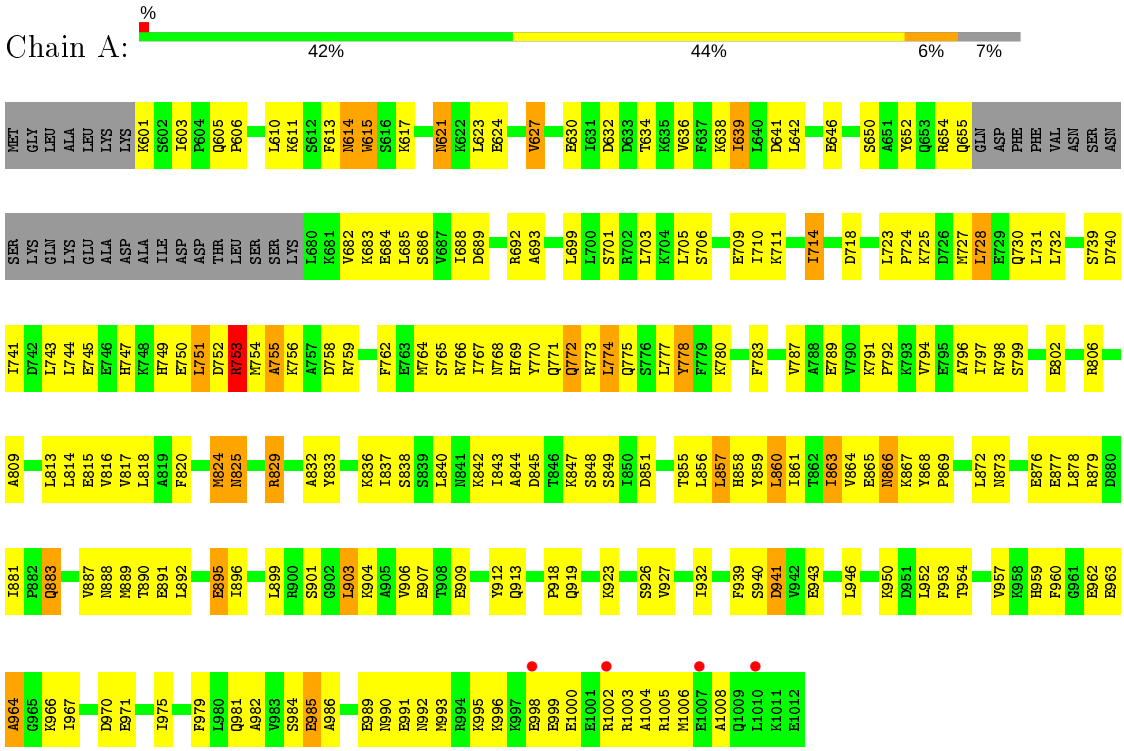
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total	O	0	0
			32	32		
2	B	35	Total	O	0	0
			35	35		
2	C	20	Total	O	0	0
			20	20		
2	D	35	Total	O	0	0
			35	35		

3 Residue-property plots (i)

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

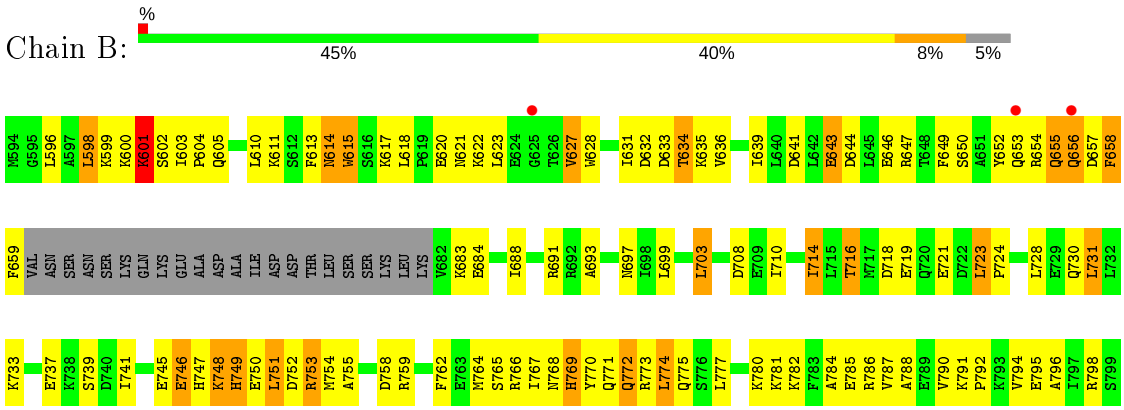
- Molecule 1: Disheveled-associated activator of morphogenesis 1

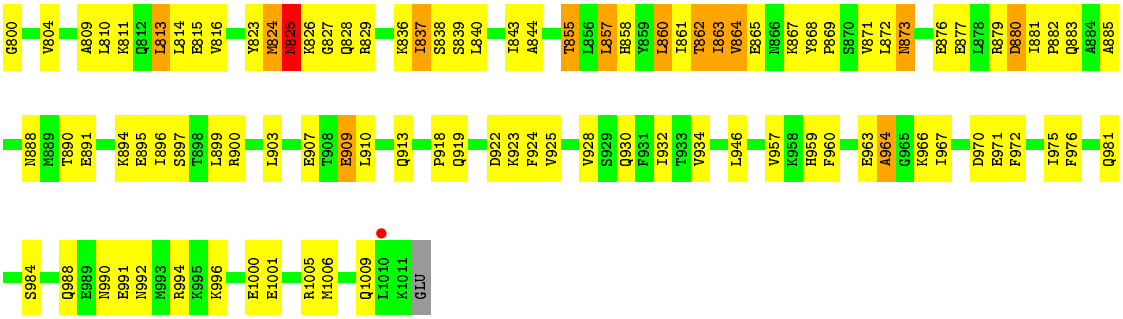
Chain A:



- Molecule 1: Disheveled-associated activator of morphogenesis 1

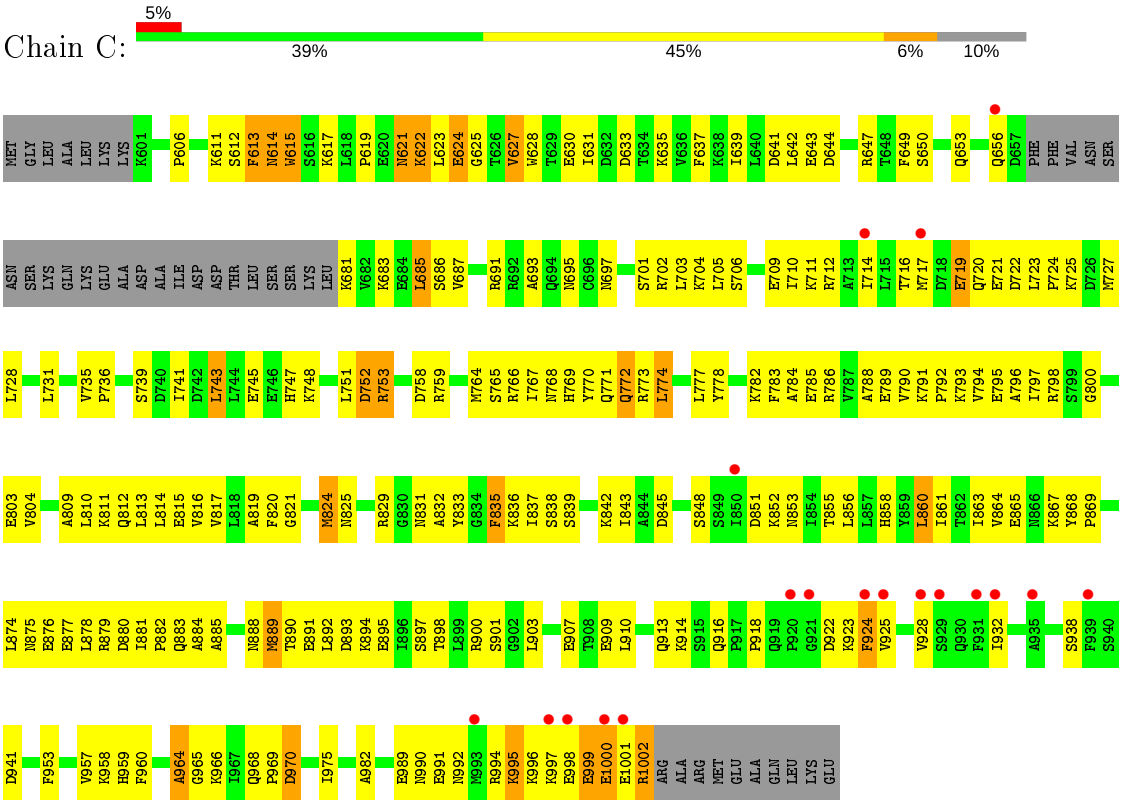
Chain B:





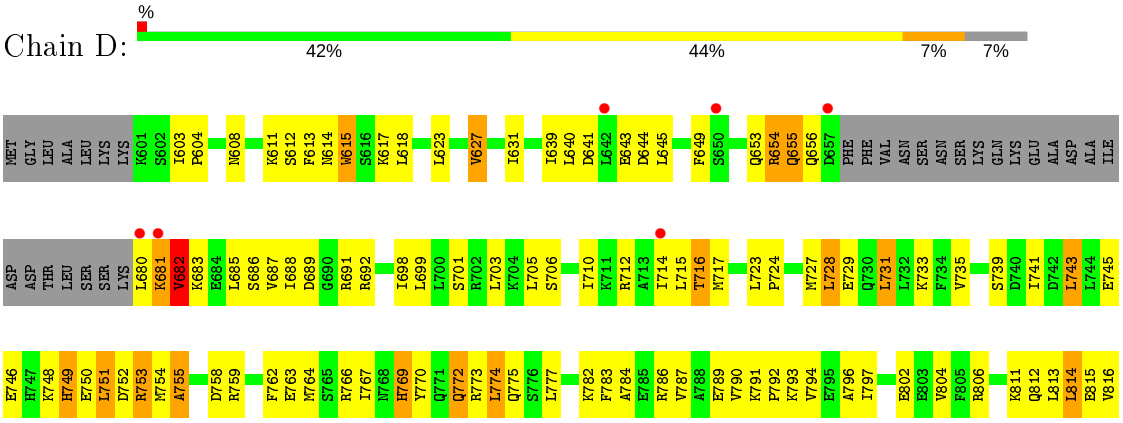
• Molecule 1: Disheveled-associated activator of morphogenesis 1

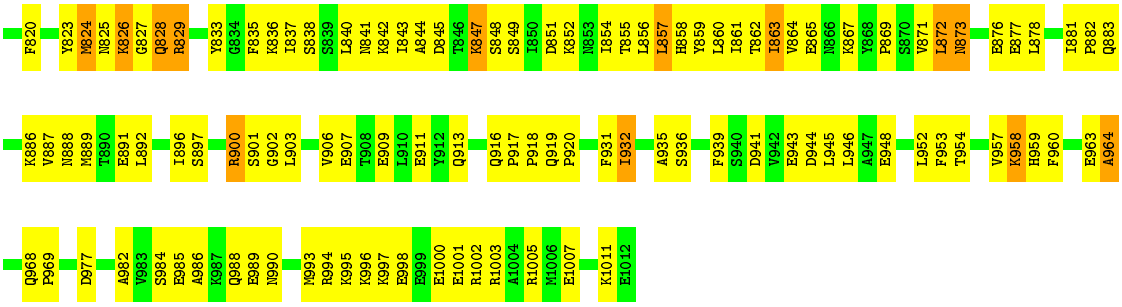
Chain C:



• Molecule 1: Disheveled-associated activator of morphogenesis 1

Chain D:




F820
Y823 M824 N825 K826 G827 Q828 R829
Y833 G834 F835 K836 I837 S838 S839 L840 N841 K842 I843 A844 D845 T846 K847 S848 S849 I850 D851 K852 N853 I854 T855 L856 L857 H858 Y859 L860 I861 T862 I863 V864 E865 N866 K867 Y868 P869 S870 V871 L872 N873
E876 E877 L878
I881 P882 Q883
K886 V887 N888 M889 T890 E891 L892
I896 S897
R900 S901 G902 L903
V906 E907 T908 E909 L910 E911 Y912 Q913
Q916 P917 P918 Q919 P920
F931 I932
A935 S936
F939 S940 D941 V942 E943 D944 L945 L946 A947 E948
L952 F953 T954
V957 K958 H959 F960
E963 A964
Q968 P969
D977
A982 Y983 S984 E985 A986 K987 Q988 E989 N990
N993 R994 K995 K996 K997 E998 E999 E1000 E1001 R1002 R1003 A1004 R1005 M1006 E1007
K1011 E1012

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.21Å 91.89Å 97.68Å 98.12° 90.32° 104.79°	Depositor
Resolution (Å)	29.82 – 2.80 48.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.8 (29.82-2.80) 86.9 (48.31-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.289 0.223 , 0.285	Depositor DCC
R_{free} test set	2471 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12750	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.45	0/3204	0.66	0/4297
1	B	0.45	0/3269	0.63	1/4384 (0.0%)
1	C	0.40	0/3128	0.61	0/4199
1	D	0.42	0/3221	0.63	1/4320 (0.0%)
All	All	0.43	0/12822	0.63	2/17200 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	682	VAL	N-CA-C	5.77	126.58	111.00
1	B	754	MET	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	778	TYR	Sidechain

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	3156	0	3193	216	0
1	B	3219	0	3258	238	0
1	C	3080	0	3105	261	0
1	D	3173	0	3205	250	0
2	A	32	0	0	4	0
2	B	35	0	0	3	0
2	C	20	0	0	7	0
2	D	35	0	0	5	0
All	All	12750	0	12761	864	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 34.

All (864) 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:D:958:LYS:HE3	1:D:964:ALA:HA	1.23	1.18
1:D:655:GLN:HG3	1:D:683:LYS:HD2	1.19	1.14
1:B:723:LEU:HB3	1:B:728:LEU:HD11	1.39	1.03
1:B:768:ASN:HD22	1:B:773:ARG:HH21	1.00	0.99
1:C:992:ASN:O	1:C:995:LYS:HG3	1.61	0.98
1:B:855:THR:H	1:B:858:HIS:HD2	1.11	0.98
1:D:855:THR:H	1:D:858:HIS:HD2	1.10	0.97
1:B:601:LYS:HD2	1:B:602:SER:H	1.27	0.96
1:D:985:GLU:O	1:D:989:GLU:HG3	1.67	0.95
1:D:655:GLN:CG	1:D:683:LYS:HD2	1.96	0.94
1:D:611:LYS:HE2	1:D:653:GLN:HE22	1.30	0.93
1:B:855:THR:HG22	1:B:858:HIS:CD2	2.03	0.93
1:C:997:LYS:HD3	1:C:998:GLU:N	1.84	0.92
1:A:627:VAL:HG13	1:B:959:HIS:NE2	1.87	0.89
1:C:959:HIS:NE2	1:D:627:VAL:HG13	1.86	0.89
1:D:855:THR:HG23	1:D:857:LEU:H	1.35	0.89
1:C:836:LYS:HG2	1:D:618:LEU:HD11	1.52	0.89
1:C:687:VAL:HG11	1:C:743:LEU:HD22	1.53	0.89
1:A:849:SER:HB2	1:B:653:GLN:NE2	1.88	0.89
1:B:772:GLN:HB2	1:B:909:GLU:HG2	1.54	0.89
1:A:855:THR:H	1:A:858:HIS:HD2	1.21	0.89
1:D:878:LEU:HB3	1:D:881:ILE:HD12	1.54	0.86
1:B:855:THR:H	1:B:858:HIS:CD2	1.94	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:897:SER:HA	1:D:900:ARG:HG2	1.58	0.85
1:C:623:LEU:HD21	1:D:833:TYR:HB3	1.58	0.85
1:C:1002:ARG:O	1:C:1002:ARG:HD2	1.76	0.85
1:C:897:SER:HA	1:C:900:ARG:HG2	1.59	0.84
1:D:855:THR:H	1:D:858:HIS:CD2	1.95	0.83
1:B:751:LEU:H	1:B:751:LEU:CD2	1.91	0.83
1:C:711:LYS:HG3	1:C:767:ILE:HD11	1.61	0.82
1:C:861:ILE:O	1:C:864:VAL:HG12	1.80	0.82
1:B:829:ARG:HA	1:B:829:ARG:NE	1.95	0.81
1:D:958:LYS:CE	1:D:964:ALA:HA	2.08	0.81
1:C:627:VAL:HG13	1:D:959:HIS:NE2	1.96	0.81
1:D:888:ASN:HD22	1:D:891:GLU:HB2	1.44	0.80
1:C:842:LYS:HD2	1:D:614:ASN:ND2	1.97	0.80
1:C:725:LYS:HB3	1:C:782:LYS:NZ	1.97	0.80
1:C:813:LEU:HD11	1:C:860:LEU:HD11	1.63	0.80
1:B:741:ILE:O	1:B:745:GLU:HG2	1.81	0.79
1:A:866:ASN:N	1:A:866:ASN:HD22	1.77	0.79
1:C:791:LYS:O	1:C:794:VAL:HG12	1.81	0.79
1:B:800:GLY:O	1:B:804:VAL:HG23	1.83	0.79
1:B:751:LEU:HD23	1:B:751:LEU:H	1.47	0.79
1:C:867:LYS:HD2	1:D:639:ILE:HG22	1.65	0.79
1:D:612:SER:OG	1:D:743:LEU:HD11	1.82	0.79
1:D:741:ILE:O	1:D:745:GLU:HG2	1.82	0.79
1:A:842:LYS:HD2	1:B:614:ASN:ND2	1.97	0.78
1:A:630:GLU:HB2	1:B:811:LYS:HE3	1.64	0.78
1:B:772:GLN:CB	1:B:909:GLU:HG2	2.13	0.78
1:B:632:ASP:OD1	1:B:634:THR:HB	1.82	0.78
1:C:709:GLU:O	1:C:712:ARG:HG2	1.84	0.78
1:D:735:VAL:HG12	1:D:770:TYR:HE1	1.48	0.78
1:C:810:LEU:O	1:C:814:LEU:HD13	1.84	0.78
1:D:829:ARG:NE	1:D:829:ARG:HA	1.99	0.77
1:A:632:ASP:OD2	1:A:634:THR:HB	1.84	0.77
1:C:786:ARG:HH12	1:C:898:THR:HG22	1.48	0.77
1:C:816:VAL:HG12	1:C:820:PHE:CE2	2.18	0.77
1:A:813:LEU:O	1:A:817:VAL:HG23	1.85	0.77
1:C:843:ILE:HA	1:D:613:PHE:HE1	1.50	0.76
1:C:723:LEU:HB3	1:C:728:LEU:HD11	1.67	0.76
1:D:753:ARG:HA	1:D:753:ARG:HE	1.51	0.76
1:D:958:LYS:HE3	1:D:964:ALA:CA	2.12	0.75
1:A:703:LEU:CD1	1:A:705:LEU:HB2	2.17	0.75
1:A:739:SER:HA	1:B:829:ARG:HD2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ASP:OD2	1:B:644:ASP:HB2	1.87	0.75
1:D:714:ILE:HD11	1:D:767:ILE:HD13	1.67	0.75
1:D:855:THR:HG23	1:D:857:LEU:N	2.01	0.75
1:A:689:ASP:OD1	1:A:692:ARG:HD3	1.87	0.75
1:C:716:THR:HG23	1:C:923:LYS:HD2	1.69	0.75
1:D:855:THR:HG22	1:D:858:HIS:CD2	2.22	0.74
1:A:751:LEU:CD2	1:A:751:LEU:H	2.00	0.74
1:C:907:GLU:HA	1:C:932:ILE:HD11	1.69	0.74
1:A:861:ILE:O	1:A:864:VAL:HG12	1.88	0.74
1:D:641:ASP:OD2	1:D:644:ASP:HB2	1.87	0.74
1:A:654:ARG:O	1:A:655:GLN:HB2	1.86	0.73
1:B:768:ASN:HD22	1:B:773:ARG:NH2	1.81	0.73
1:A:873:ASN:O	1:A:877:GLU:HG2	1.87	0.73
1:C:894:LYS:HA	2:C:93:HOH:O	1.89	0.73
1:A:855:THR:HG22	1:A:858:HIS:CD2	2.23	0.73
1:A:751:LEU:H	1:A:751:LEU:HD23	1.54	0.72
1:D:681:LYS:O	1:D:682:VAL:HG13	1.90	0.72
1:C:918:PRO:HB2	2:C:121:HOH:O	1.89	0.72
1:A:630:GLU:HB2	1:B:811:LYS:CE	2.20	0.72
1:C:804:VAL:HG22	1:C:881:ILE:HD11	1.71	0.72
1:A:855:THR:HG23	1:A:857:LEU:H	1.54	0.72
1:B:869:PRO:O	1:B:872:LEU:HD23	1.90	0.72
1:A:743:LEU:HG	1:B:829:ARG:HG3	1.72	0.72
1:C:897:SER:HA	1:C:900:ARG:CG	2.19	0.71
1:D:699:LEU:HD21	1:D:731:LEU:HD12	1.72	0.71
1:C:656:GLN:CD	1:D:852:LYS:HE2	2.10	0.71
1:B:873:ASN:O	1:B:877:GLU:HG2	1.90	0.71
1:C:769:HIS:O	1:C:772:GLN:HG2	1.90	0.71
1:C:816:VAL:HG12	1:C:820:PHE:HE2	1.54	0.71
1:D:611:LYS:HE2	1:D:653:GLN:NE2	2.05	0.71
1:C:867:LYS:HD2	1:D:639:ILE:CG2	2.21	0.71
1:B:731:LEU:HB3	1:B:774:LEU:HD11	1.73	0.71
1:B:751:LEU:HD23	1:B:751:LEU:N	2.06	0.71
1:D:796:ALA:HB1	1:D:883:GLN:O	1.90	0.71
1:B:601:LYS:CD	1:B:602:SER:H	2.03	0.70
1:C:888:ASN:ND2	1:C:891:GLU:HB2	2.06	0.70
1:D:703:LEU:HD22	1:D:705:LEU:HB2	1.72	0.70
1:A:959:HIS:NE2	1:B:627:VAL:HG13	2.05	0.70
1:C:725:LYS:HB3	1:C:782:LYS:HZ2	1.55	0.70
1:A:833:TYR:HB3	1:B:623:LEU:HD21	1.73	0.70
1:C:809:ALA:HB3	1:C:874:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:ILE:HG21	1:B:764:MET:HE2	1.73	0.70
1:B:786:ARG:O	1:B:790:VAL:HG23	1.91	0.70
1:A:833:TYR:CB	1:B:623:LEU:HD21	2.22	0.69
1:C:728:LEU:HD21	1:C:777:LEU:HG	1.74	0.69
1:D:873:ASN:O	1:D:877:GLU:HG2	1.93	0.69
1:D:861:ILE:O	1:D:864:VAL:HG12	1.92	0.69
1:B:991:GLU:HG2	1:B:994:ARG:NH2	2.09	0.68
1:A:772:GLN:N	1:A:772:GLN:HE21	1.91	0.68
1:A:855:THR:H	1:A:858:HIS:CD2	2.07	0.68
1:D:888:ASN:ND2	1:D:891:GLU:H	1.90	0.68
1:A:654:ARG:O	1:A:655:GLN:CB	2.42	0.68
1:A:848:SER:HB3	1:A:851:ASP:O	1.94	0.68
1:A:849:SER:HB2	1:B:653:GLN:CD	2.14	0.68
1:A:842:LYS:HD2	1:B:614:ASN:HD22	1.57	0.67
1:D:828:GLN:HE22	1:D:829:ARG:NH2	1.92	0.67
1:A:838:SER:HB2	2:A:7:HOH:O	1.93	0.67
1:A:992:ASN:O	1:A:996:LYS:HG3	1.94	0.67
1:B:796:ALA:HB1	1:B:883:GLN:O	1.94	0.67
1:A:866:ASN:N	1:A:866:ASN:ND2	2.43	0.67
1:A:985:GLU:O	1:A:989:GLU:HG3	1.94	0.67
1:A:768:ASN:ND2	1:A:913:GLN:HE22	1.93	0.67
1:C:909:GLU:HG3	1:C:924:PHE:CZ	2.30	0.67
1:C:627:VAL:HG13	1:D:959:HIS:CD2	2.30	0.67
1:A:772:GLN:HG3	1:A:909:GLU:OE1	1.93	0.66
1:A:769:HIS:O	1:A:772:GLN:HG2	1.95	0.66
1:A:639:ILE:HD11	1:B:868:TYR:OH	1.94	0.66
1:B:855:THR:N	1:B:858:HIS:HD2	1.91	0.66
1:B:930:GLN:O	1:B:934:VAL:HG23	1.95	0.66
1:C:644:ASP:O	1:C:647:ARG:HG2	1.96	0.66
1:C:989:GLU:HA	1:C:992:ASN:ND2	2.10	0.66
1:C:999:GLU:O	1:C:1002:ARG:HB3	1.96	0.66
1:A:861:ILE:O	1:A:865:GLU:HG3	1.96	0.66
1:A:878:LEU:HB3	1:A:881:ILE:HD12	1.78	0.66
1:C:741:ILE:O	1:C:745:GLU:HG2	1.96	0.66
1:D:907:GLU:O	1:D:911:GLU:HG2	1.96	0.66
1:B:610:LEU:HD21	1:B:646:GLU:HA	1.77	0.66
1:C:685:LEU:HD11	1:C:747:HIS:CG	2.31	0.66
1:C:703:LEU:HD11	1:C:731:LEU:HD21	1.78	0.66
1:C:796:ALA:HB1	1:C:883:GLN:O	1.96	0.66
1:D:731:LEU:HB3	1:D:774:LEU:HD11	1.77	0.65
1:D:844:ALA:O	1:D:847:LYS:HE3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:997:LYS:NZ	1:C:998:GLU:HG2	2.11	0.65
1:D:814:LEU:HD12	1:D:835:PHE:CZ	2.31	0.65
1:C:716:THR:HG21	1:C:719:GLU:HB3	1.77	0.65
1:D:745:GLU:O	1:D:748:LYS:HG3	1.97	0.65
1:B:714:ILE:C	1:B:714:ILE:HD12	2.18	0.65
1:C:991:GLU:HG3	1:C:994:ARG:NH1	2.11	0.65
1:C:953:PHE:O	1:C:957:VAL:HG23	1.96	0.64
1:D:931:PHE:CE1	1:D:935:ALA:HB2	2.32	0.64
1:C:716:THR:CG2	1:C:719:GLU:HB3	2.26	0.64
1:B:748:LYS:O	1:B:751:LEU:HD22	1.97	0.64
1:D:826:LYS:HE3	1:D:827:GLY:N	2.11	0.64
1:A:773:ARG:NH2	1:A:913:GLN:NE2	2.46	0.64
1:A:843:ILE:HG12	1:B:613:PHE:CZ	2.32	0.64
1:B:764:MET:HE3	1:B:770:TYR:CE2	2.33	0.64
1:D:855:THR:HG22	1:D:858:HIS:CG	2.33	0.64
1:D:996:LYS:O	1:D:1000:GLU:HG3	1.98	0.63
1:B:768:ASN:ND2	1:B:773:ARG:HH21	1.84	0.63
1:A:906:VAL:HG12	1:A:932:ILE:HD11	1.80	0.63
1:C:687:VAL:HG11	1:C:743:LEU:CD2	2.26	0.63
1:C:627:VAL:HG22	1:D:959:HIS:O	1.98	0.63
1:A:753:ARG:HA	1:A:753:ARG:HH11	1.63	0.63
1:C:888:ASN:HD22	1:C:891:GLU:HB2	1.63	0.63
1:B:618:LEU:HD23	1:B:623:LEU:HD12	1.80	0.63
1:A:613:PHE:HB3	1:B:825:ASN:OD1	1.99	0.63
1:D:613:PHE:CE2	1:D:615:TRP:HB3	2.33	0.63
1:D:852:LYS:HG3	2:D:69:HOH:O	1.96	0.63
1:C:804:VAL:HG12	1:C:960:PHE:CE1	2.34	0.62
1:D:735:VAL:HG12	1:D:770:TYR:CE1	2.32	0.62
1:A:796:ALA:HB1	1:A:883:GLN:O	2.00	0.62
1:C:783:PHE:N	2:C:15:HOH:O	2.33	0.62
1:C:784:ALA:HB3	2:C:113:HOH:O	1.99	0.62
1:A:706:SER:OG	1:A:709:GLU:HG3	1.99	0.62
1:A:741:ILE:O	1:A:745:GLU:HG2	1.99	0.62
1:B:724:PRO:O	1:B:728:LEU:HD13	1.99	0.62
1:C:741:ILE:CD1	1:C:765:SER:HB2	2.30	0.61
1:C:994:ARG:HB3	1:C:994:ARG:NH1	2.15	0.61
1:D:703:LEU:O	1:D:703:LEU:HD23	1.99	0.61
1:A:768:ASN:HD22	1:A:913:GLN:HE22	1.48	0.61
1:A:802:GLU:HG2	1:A:806:ARG:HD2	1.81	0.61
1:C:888:ASN:ND2	1:C:891:GLU:CB	2.63	0.61
1:D:1003:ARG:O	1:D:1007:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:682:VAL:O	1:D:683:LYS:HD3	1.99	0.61
1:D:804:VAL:HG12	1:D:960:PHE:CE1	2.35	0.61
1:B:791:LYS:O	1:B:794:VAL:HG12	2.01	0.61
1:C:848:SER:HB2	1:C:851:ASP:O	2.01	0.61
1:D:751:LEU:H	1:D:751:LEU:HD23	1.64	0.61
1:C:722:ASP:O	1:C:724:PRO:HD3	1.99	0.61
1:D:655:GLN:HG3	1:D:683:LYS:CD	2.11	0.61
1:C:803:GLU:OE1	1:C:880:ASP:HB2	2.01	0.61
1:C:815:GLU:HB2	1:D:631:ILE:HG23	1.82	0.61
1:A:732:LEU:HD23	1:A:774:LEU:HD13	1.83	0.61
1:A:867:LYS:HD3	1:B:639:ILE:HG22	1.82	0.61
1:B:794:VAL:HG21	1:B:946:LEU:HA	1.83	0.61
1:D:857:LEU:O	1:D:861:ILE:HG13	2.01	0.60
1:B:868:TYR:N	1:B:869:PRO:HD3	2.16	0.60
1:C:821:GLY:HA3	1:D:615:TRP:CZ3	2.36	0.60
1:C:656:GLN:OE1	1:D:852:LYS:HE2	2.01	0.60
1:C:739:SER:HB2	1:D:829:ARG:HD2	1.83	0.60
1:D:714:ILE:HD12	1:D:715:LEU:N	2.16	0.60
1:A:603:ILE:HG22	1:A:605:GLN:HG2	1.84	0.60
1:C:723:LEU:HB3	1:C:728:LEU:CD1	2.31	0.60
1:A:728:LEU:HD21	1:A:777:LEU:HG	1.82	0.60
1:C:892:LEU:C	1:C:892:LEU:HD23	2.22	0.60
1:C:842:LYS:HD2	1:D:614:ASN:HD21	1.67	0.60
1:C:724:PRO:O	1:C:728:LEU:HD13	2.02	0.60
1:C:711:LYS:HG3	1:C:767:ILE:CD1	2.31	0.59
1:A:703:LEU:HD13	1:A:705:LEU:HB2	1.83	0.59
1:B:924:PHE:CZ	1:B:928:VAL:HG21	2.37	0.59
1:D:613:PHE:O	1:D:614:ASN:HB3	2.01	0.59
1:A:710:ILE:HG21	1:A:764:MET:HE1	1.84	0.59
1:A:843:ILE:HA	1:B:613:PHE:HE1	1.66	0.59
1:A:769:HIS:HD2	1:A:909:GLU:OE1	1.85	0.59
1:B:786:ARG:HB3	1:B:899:LEU:HD21	1.85	0.59
1:B:900:ARG:NH1	1:B:900:ARG:HB2	2.18	0.59
1:C:773:ARG:NH1	1:C:922:ASP:OD1	2.36	0.59
1:D:998:GLU:O	1:D:1001:GLU:HB2	2.03	0.59
1:D:729:GLU:O	1:D:733:LYS:HE2	2.03	0.59
1:B:714:ILE:HD11	1:B:767:ILE:HG21	1.83	0.59
1:D:855:THR:HG22	1:D:858:HIS:H	1.68	0.59
1:B:613:PHE:O	1:B:614:ASN:HB3	2.03	0.58
1:B:688:ILE:HG22	1:B:693:ALA:HB2	1.85	0.58
1:C:800:GLY:O	1:C:804:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:LYS:CE	1:D:653:GLN:HE22	2.09	0.58
1:D:751:LEU:H	1:D:751:LEU:CD2	2.16	0.58
1:A:769:HIS:HB3	1:A:772:GLN:HG2	1.85	0.58
1:B:596:LEU:O	1:B:599:LYS:HB2	2.02	0.58
1:B:714:ILE:O	1:B:714:ILE:HD12	2.02	0.58
1:A:652:TYR:HA	1:A:684:GLU:O	2.03	0.58
1:C:706:SER:OG	1:C:709:GLU:HG3	2.03	0.58
1:C:745:GLU:OE2	1:C:766:ARG:NH1	2.36	0.58
1:A:843:ILE:HA	1:B:613:PHE:CE1	2.39	0.58
1:A:772:GLN:N	1:A:772:GLN:NE2	2.51	0.58
1:A:889:MET:HE2	1:A:950:LYS:HE3	1.85	0.58
1:C:809:ALA:CB	1:C:874:LEU:HD13	2.33	0.58
1:C:852:LYS:HZ1	1:D:656:GLN:HA	1.69	0.58
1:B:828:GLN:O	1:B:828:GLN:HG2	2.03	0.58
1:B:879:ARG:HG3	1:B:880:ASP:OD1	2.04	0.58
1:C:621:ASN:ND2	1:C:622:LYS:HD2	2.18	0.58
1:A:762:PHE:CE1	1:A:766:ARG:HD3	2.39	0.57
1:C:959:HIS:O	1:D:627:VAL:HG22	2.03	0.57
1:A:848:SER:HA	1:B:649:PHE:CD2	2.39	0.57
1:B:777:LEU:HD11	1:B:781:LYS:HE3	1.85	0.57
1:B:810:LEU:O	1:B:814:LEU:HD13	2.03	0.57
1:C:863:ILE:HD12	1:C:863:ILE:C	2.24	0.57
1:B:745:GLU:O	1:B:748:LYS:HG2	2.04	0.57
1:B:829:ARG:HA	1:B:829:ARG:CZ	2.34	0.57
1:C:892:LEU:HA	1:C:895:GLU:OE2	2.05	0.57
1:C:964:ALA:O	1:C:966:LYS:N	2.37	0.57
1:C:748:LYS:HA	1:C:751:LEU:HD21	1.86	0.57
1:D:769:HIS:CD2	1:D:772:GLN:HG3	2.39	0.57
1:D:842:LYS:O	1:D:845:ASP:HB2	2.03	0.57
1:D:883:GLN:NE2	1:D:886:LYS:NZ	2.53	0.57
1:A:617:LYS:NZ	1:B:829:ARG:HH21	2.02	0.57
1:B:782:LYS:HG2	1:B:785:GLU:OE1	2.05	0.57
1:C:836:LYS:HG2	1:D:618:LEU:CD1	2.30	0.57
1:A:918:PRO:O	1:A:919:GLN:HG3	2.05	0.57
1:A:998:GLU:HG3	1:A:1002:ARG:CZ	2.35	0.57
1:B:862:THR:HG23	1:B:990:ASN:ND2	2.20	0.57
1:C:695:ASN:N	1:C:695:ASN:HD22	2.01	0.57
1:B:655:GLN:HG2	1:B:753:ARG:NH2	2.19	0.57
1:C:621:ASN:ND2	1:C:622:LYS:NZ	2.52	0.57
1:C:913:GLN:HG3	1:C:924:PHE:CE2	2.39	0.57
1:D:753:ARG:NE	1:D:753:ARG:HA	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:LEU:N	1:A:751:LEU:HD23	2.20	0.57
1:B:873:ASN:HA	1:B:876:GLU:OE2	2.05	0.57
1:D:723:LEU:HB3	1:D:728:LEU:CD1	2.35	0.57
1:D:855:THR:CG2	1:D:858:HIS:H	2.17	0.56
1:A:773:ARG:NH2	1:A:913:GLN:HE22	2.03	0.56
1:B:910:LEU:HD23	1:B:932:ILE:HD12	1.86	0.56
1:C:991:GLU:HG3	1:C:994:ARG:HH12	1.70	0.56
1:C:815:GLU:CB	1:D:631:ILE:HG23	2.36	0.56
1:C:851:ASP:OD2	1:C:853:ASN:HB2	2.05	0.56
1:C:832:ALA:HB2	1:D:617:LYS:HD2	1.87	0.56
1:D:873:ASN:HA	1:D:876:GLU:OE2	2.04	0.56
1:D:790:VAL:HG11	1:D:896:ILE:HD11	1.87	0.56
1:D:900:ARG:NH2	1:D:943:GLU:OE2	2.37	0.56
1:C:860:LEU:O	1:C:864:VAL:HB	2.06	0.56
1:D:829:ARG:HA	1:D:829:ARG:CZ	2.35	0.56
1:D:685:LEU:HD23	1:D:686:SER:N	2.20	0.56
1:D:968:GLN:HB3	1:D:969:PRO:HD2	1.87	0.56
1:A:688:ILE:HG22	1:A:693:ALA:HB2	1.86	0.56
1:B:963:GLU:O	1:B:964:ALA:O	2.22	0.56
1:C:997:LYS:HZ3	1:C:998:GLU:HG2	1.70	0.56
1:D:855:THR:N	1:D:858:HIS:HD2	1.92	0.56
1:D:892:LEU:HD23	1:D:892:LEU:O	2.06	0.56
1:B:600:LYS:HG2	1:B:601:LYS:H	1.71	0.56
1:B:869:PRO:HA	1:B:872:LEU:HD23	1.86	0.56
1:D:900:ARG:HH11	1:D:900:ARG:CB	2.19	0.56
1:B:601:LYS:HD2	1:B:602:SER:OG	2.06	0.56
1:A:847:LYS:O	1:B:611:LYS:HD2	2.06	0.56
1:C:705:LEU:HA	1:C:709:GLU:OE1	2.06	0.56
1:A:966:LYS:HB3	2:A:27:HOH:O	2.05	0.56
1:B:784:ALA:O	1:B:787:VAL:HG12	2.05	0.56
1:A:723:LEU:HB3	1:A:728:LEU:HD13	1.88	0.55
1:B:777:LEU:O	1:B:781:LYS:HG2	2.06	0.55
1:C:741:ILE:HG12	1:C:765:SER:HB2	1.87	0.55
1:A:797:ILE:HD11	1:A:887:VAL:HG11	1.88	0.55
1:A:889:MET:HE3	1:A:892:LEU:HD13	1.89	0.55
1:D:654:ARG:HA	1:D:683:LYS:HG3	1.87	0.55
1:D:687:VAL:HG23	1:D:688:ILE:HD12	1.88	0.55
1:C:769:HIS:HB3	1:C:772:GLN:CG	2.36	0.55
1:A:844:ALA:O	1:A:855:THR:OG1	2.24	0.55
1:C:649:PHE:CD2	1:D:848:SER:HA	2.42	0.55
1:A:762:PHE:O	1:A:766:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:MET:CE	1:A:892:LEU:HD13	2.36	0.55
1:B:750:GLU:C	1:B:752:ASP:H	2.10	0.55
1:D:723:LEU:HB3	1:D:728:LEU:HD13	1.88	0.55
1:A:699:LEU:HD21	1:A:731:LEU:HD12	1.89	0.55
1:B:861:ILE:O	1:B:865:GLU:HG3	2.06	0.55
1:B:604:PRO:HD2	2:B:43:HOH:O	2.06	0.55
1:A:611:LYS:HE3	1:A:650:SER:O	2.07	0.55
1:C:721:GLU:O	1:C:721:GLU:HG3	2.07	0.55
1:B:598:LEU:N	1:B:598:LEU:HD23	2.22	0.55
1:B:855:THR:HG23	1:B:857:LEU:H	1.71	0.55
1:B:913:GLN:HG3	1:B:924:PHE:CD2	2.42	0.55
1:A:845:ASP:OD1	1:B:691:ARG:HB2	2.08	0.54
1:A:865:GLU:C	1:A:866:ASN:HD22	2.10	0.54
1:A:892:LEU:HD23	1:A:892:LEU:C	2.27	0.54
1:D:824:MET:CE	1:D:856:LEU:HD22	2.37	0.54
1:D:945:LEU:O	1:D:948:GLU:HB3	2.08	0.54
1:A:849:SER:HA	1:B:653:GLN:HG3	1.89	0.54
1:D:888:ASN:HD22	1:D:891:GLU:CB	2.16	0.54
1:A:764:MET:HE2	1:A:770:TYR:CE2	2.42	0.54
1:A:820:PHE:O	1:A:824:MET:CG	2.55	0.54
1:C:888:ASN:HD22	1:C:891:GLU:CB	2.20	0.54
1:B:752:ASP:O	1:B:753:ARG:C	2.46	0.54
1:D:703:LEU:HD21	1:D:705:LEU:HD12	1.90	0.54
1:D:828:GLN:HE22	1:D:829:ARG:CZ	2.20	0.54
1:C:612:SER:HB3	1:C:743:LEU:HD11	1.89	0.54
1:A:747:HIS:HA	1:A:749:HIS:CE1	2.41	0.54
1:A:855:THR:HG23	1:A:857:LEU:N	2.20	0.54
1:A:773:ARG:HH21	1:A:913:GLN:HE22	1.56	0.54
1:B:750:GLU:C	1:B:752:ASP:N	2.61	0.54
1:D:786:ARG:O	1:D:789:GLU:HG2	2.08	0.54
1:A:725:LYS:HG2	2:A:19:HOH:O	2.08	0.54
1:B:924:PHE:O	1:B:928:VAL:HG23	2.08	0.54
1:C:868:TYR:N	1:C:869:PRO:HD3	2.23	0.54
1:C:913:GLN:HG3	1:C:924:PHE:CD2	2.42	0.54
1:D:918:PRO:O	1:D:919:GLN:HG2	2.08	0.54
1:A:771:GLN:HE22	1:A:775:GLN:HG3	1.73	0.54
1:B:1006:MET:HA	1:B:1009:GLN:HB3	1.90	0.54
1:C:613:PHE:O	1:C:613:PHE:HD1	1.91	0.54
1:C:731:LEU:HB3	1:C:774:LEU:HD11	1.90	0.54
1:C:813:LEU:O	1:C:817:VAL:HG23	2.07	0.54
1:D:889:MET:HE3	1:D:889:MET:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:LYS:HA	2:A:29:HOH:O	2.07	0.53
1:B:769:HIS:O	1:B:773:ARG:CG	2.56	0.53
1:C:860:LEU:O	1:C:860:LEU:HD22	2.08	0.53
1:B:804:VAL:HG12	1:B:960:PHE:CE1	2.42	0.53
1:C:852:LYS:NZ	1:D:656:GLN:HA	2.24	0.53
1:A:873:ASN:HA	1:A:876:GLU:OE1	2.08	0.53
1:B:910:LEU:HA	1:B:924:PHE:HE2	1.74	0.53
1:C:891:GLU:O	1:C:895:GLU:HG3	2.09	0.53
1:B:881:ILE:HB	1:B:882:PRO:HD3	1.89	0.53
1:D:784:ALA:O	1:D:787:VAL:HG12	2.09	0.53
1:C:794:VAL:HG13	1:C:795:GLU:N	2.24	0.53
1:A:848:SER:HA	1:B:649:PHE:CE2	2.43	0.53
1:C:910:LEU:HA	1:C:924:PHE:HE2	1.73	0.53
1:C:994:ARG:HB3	1:C:994:ARG:HH11	1.73	0.53
1:D:712:ARG:O	1:D:716:THR:OG1	2.27	0.53
1:D:764:MET:CE	1:D:770:TYR:CE2	2.92	0.53
1:B:795:GLU:CD	1:B:798:ARG:HE	2.12	0.52
1:C:748:LYS:O	1:C:751:LEU:HG	2.09	0.52
1:C:910:LEU:O	1:C:914:LYS:HG3	2.10	0.52
1:A:718:ASP:OD2	1:A:723:LEU:HB2	2.10	0.52
1:A:889:MET:CE	1:A:950:LYS:HE3	2.39	0.52
1:C:642:LEU:HD13	1:D:823:TYR:CE1	2.44	0.52
1:D:939:PHE:C	1:D:941:ASP:N	2.63	0.52
1:D:1007:GLU:O	1:D:1011:LYS:HB2	2.10	0.52
1:A:682:VAL:HG12	1:A:683:LYS:N	2.24	0.52
1:B:693:ALA:O	1:B:697:ASN:ND2	2.42	0.52
1:D:820:PHE:CE2	1:D:860:LEU:HD23	2.45	0.52
1:D:838:SER:HB2	2:D:106:HOH:O	2.09	0.52
1:A:1002:ARG:O	1:A:1005:ARG:HB3	2.09	0.52
1:C:693:ALA:O	1:C:697:ASN:ND2	2.43	0.52
1:D:900:ARG:NH1	1:D:900:ARG:HB3	2.23	0.52
1:C:621:ASN:HD22	1:C:622:LYS:HD2	1.72	0.52
1:C:719:GLU:OE2	1:C:720:GLN:HG2	2.10	0.52
1:C:716:THR:CG2	1:C:923:LYS:HD2	2.39	0.52
1:D:791:LYS:N	1:D:792:PRO:HD2	2.25	0.52
1:A:601:LYS:O	1:A:603:ILE:HG13	2.09	0.52
1:A:791:LYS:N	1:A:792:PRO:HD2	2.25	0.52
1:A:849:SER:HB2	1:B:653:GLN:CG	2.40	0.52
1:A:832:ALA:HB2	1:B:617:LYS:HD2	1.92	0.52
1:B:699:LEU:O	1:B:699:LEU:HD12	2.10	0.52
1:B:751:LEU:HG	1:B:759:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:794:VAL:CG2	1:B:946:LEU:HA	2.40	0.52
1:D:953:PHE:O	1:D:957:VAL:HG23	2.09	0.52
1:B:988:GLN:NE2	1:B:992:ASN:OD1	2.42	0.52
1:C:924:PHE:CE1	1:C:928:VAL:HG21	2.45	0.52
1:D:837:ILE:O	1:D:840:LEU:HG	2.10	0.52
1:A:739:SER:CA	1:B:829:ARG:HD2	2.38	0.52
1:C:768:ASN:O	1:C:773:ARG:NH2	2.36	0.52
1:D:900:ARG:HG3	1:D:901:SER:N	2.25	0.52
1:A:744:LEU:HD13	1:A:762:PHE:HB2	1.92	0.51
1:C:720:GLN:O	1:C:721:GLU:HB3	2.10	0.51
1:D:963:GLU:O	1:D:964:ALA:O	2.29	0.51
1:D:703:LEU:CD2	1:D:705:LEU:HB2	2.39	0.51
1:A:710:ILE:CG2	1:A:764:MET:HE1	2.40	0.51
1:A:769:HIS:CD2	1:A:772:GLN:HG3	2.44	0.51
1:B:924:PHE:CE2	1:B:928:VAL:HG21	2.45	0.51
1:C:804:VAL:CG2	1:C:881:ILE:HD11	2.40	0.51
1:A:728:LEU:HD23	1:A:778:TYR:HA	1.91	0.51
1:A:923:LYS:HG2	1:A:927:VAL:HG23	1.91	0.51
1:A:959:HIS:CD2	1:B:627:VAL:HG13	2.45	0.51
1:C:644:ASP:HA	1:C:647:ARG:NH1	2.25	0.51
1:A:685:LEU:HD23	1:A:754:MET:HG3	1.91	0.51
1:B:786:ARG:CB	1:B:899:LEU:HD21	2.40	0.51
1:B:844:ALA:O	1:B:855:THR:OG1	2.29	0.51
1:B:907:GLU:HG2	1:B:932:ILE:HD13	1.92	0.51
1:C:613:PHE:CD1	1:C:613:PHE:C	2.82	0.51
1:D:698:ILE:O	1:D:701:SER:OG	2.26	0.51
1:C:617:LYS:NZ	1:D:829:ARG:HH21	2.08	0.51
1:A:891:GLU:O	1:A:895:GLU:HG2	2.11	0.51
1:C:816:VAL:O	1:C:819:ALA:HB3	2.11	0.51
1:D:863:ILE:HG13	1:D:864:VAL:N	2.25	0.51
1:A:768:ASN:ND2	1:A:913:GLN:NE2	2.59	0.51
1:D:828:GLN:HE22	1:D:829:ARG:HH22	1.59	0.51
1:A:1006:MET:O	1:A:1006:MET:HG2	2.11	0.50
1:A:611:LYS:HD3	1:A:686:SER:O	2.11	0.50
1:B:650:SER:HB3	1:B:653:GLN:HE21	1.76	0.50
1:B:751:LEU:HG	1:B:759:ARG:NH1	2.26	0.50
1:B:876:GLU:OE1	1:B:876:GLU:N	2.44	0.50
1:C:831:ASN:OD1	1:D:603:ILE:HD13	2.11	0.50
1:A:627:VAL:HG13	1:B:959:HIS:CD2	2.45	0.50
1:A:967:ILE:HD11	1:A:971:GLU:CG	2.41	0.50
1:D:688:ILE:HD13	1:D:758:ASP:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ILE:CD1	1:A:770:TYR:HD2	2.24	0.50
1:B:963:GLU:HG2	1:B:964:ALA:N	2.26	0.50
1:D:772:GLN:HB2	1:D:909:GLU:CD	2.32	0.50
1:B:790:VAL:HG11	1:B:896:ILE:HD11	1.94	0.50
1:D:783:PHE:O	1:D:787:VAL:HG12	2.11	0.50
1:B:620:GLU:O	1:B:623:LEU:HB2	2.12	0.50
1:A:959:HIS:O	1:B:627:VAL:HG22	2.12	0.50
1:B:791:LYS:N	1:B:792:PRO:HD2	2.27	0.50
1:C:843:ILE:HA	1:D:613:PHE:CE1	2.39	0.50
1:D:688:ILE:HB	1:D:758:ASP:OD1	2.10	0.50
1:A:752:ASP:O	1:A:753:ARG:C	2.49	0.50
1:B:918:PRO:O	1:B:919:GLN:HG3	2.11	0.50
1:C:704:LYS:O	1:C:705:LEU:HD23	2.11	0.50
1:D:764:MET:HE3	1:D:770:TYR:CE2	2.46	0.50
1:D:840:LEU:O	1:D:843:ILE:HG13	2.12	0.50
1:D:878:LEU:HD22	1:D:881:ILE:HD11	1.94	0.50
1:D:773:ARG:NH2	1:D:913:GLN:HE22	2.10	0.50
1:B:751:LEU:HD12	1:B:759:ARG:NH1	2.27	0.50
1:A:873:ASN:HA	1:A:876:GLU:CD	2.31	0.50
1:C:621:ASN:HD21	1:C:622:LYS:NZ	2.10	0.50
1:C:624:GLU:OE1	1:C:625:GLY:N	2.43	0.50
1:C:701:SER:O	1:C:704:LYS:HG3	2.12	0.50
1:D:820:PHE:CD2	1:D:860:LEU:HD23	2.47	0.50
1:D:752:ASP:O	1:D:753:ARG:C	2.50	0.50
1:A:840:LEU:HD13	1:A:979:PHE:CD1	2.47	0.49
1:A:918:PRO:C	1:A:919:GLN:HG3	2.32	0.49
1:C:717:MET:HE1	1:C:924:PHE:HD1	1.77	0.49
1:D:769:HIS:O	1:D:772:GLN:HG2	2.12	0.49
1:C:691:ARG:HD2	1:D:845:ASP:OD1	2.12	0.49
1:B:891:GLU:HG2	1:B:895:GLU:OE2	2.12	0.49
1:B:837:ILE:HG21	1:B:976:PHE:CZ	2.47	0.49
1:D:655:GLN:CD	1:D:683:LYS:HD2	2.33	0.49
1:D:864:VAL:CG1	1:D:865:GLU:N	2.74	0.49
1:A:699:LEU:HD21	1:A:731:LEU:CD1	2.42	0.49
1:A:741:ILE:HG12	1:A:765:SER:HB2	1.93	0.49
1:A:824:MET:HE3	1:A:856:LEU:HD21	1.95	0.49
1:B:996:LYS:O	1:B:1000:GLU:HG3	2.12	0.49
1:C:768:ASN:HD21	1:C:916:GLN:HE22	1.59	0.49
1:C:889:MET:HB3	1:C:968:GLN:OE1	2.13	0.49
1:C:992:ASN:HA	1:C:995:LYS:CG	2.42	0.49
1:A:772:GLN:H	1:A:772:GLN:NE2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:LEU:CG	1:B:759:ARG:NH1	2.75	0.49
1:A:617:LYS:HZ1	1:B:829:ARG:HH21	1.59	0.49
1:B:957:VAL:HA	1:B:972:PHE:CE1	2.48	0.49
1:A:613:PHE:CE2	1:A:615:TRP:HB3	2.48	0.49
1:B:863:ILE:HD12	1:B:863:ILE:C	2.33	0.49
1:D:854:ILE:HD11	1:D:993:MET:CE	2.43	0.49
1:A:868:TYR:N	1:A:869:PRO:HD3	2.27	0.49
1:A:950:LYS:O	1:A:954:THR:HG23	2.12	0.49
1:C:992:ASN:C	1:C:995:LYS:HG3	2.32	0.49
1:D:769:HIS:CG	1:D:772:GLN:HG3	2.47	0.49
1:C:613:PHE:CZ	1:D:843:ILE:HG12	2.47	0.49
1:A:999:GLU:HG2	1:A:1003:ARG:HG3	1.94	0.49
1:A:859:TYR:CE2	1:A:863:ILE:HG21	2.48	0.49
1:A:957:VAL:CG1	1:A:962:GLU:HB2	2.43	0.49
1:C:785:GLU:O	1:C:789:GLU:HG3	2.13	0.49
1:D:828:GLN:O	1:D:828:GLN:CD	2.52	0.49
1:A:627:VAL:HG22	1:B:959:HIS:O	2.13	0.48
1:C:745:GLU:OE1	1:C:748:LYS:HE2	2.13	0.48
1:D:813:LEU:HD13	1:D:813:LEU:O	2.12	0.48
1:A:892:LEU:HD23	1:A:892:LEU:O	2.13	0.48
1:B:598:LEU:HD11	1:B:620:GLU:HB3	1.95	0.48
1:B:703:LEU:O	1:B:703:LEU:HD23	2.12	0.48
1:A:858:HIS:ND1	1:A:986:ALA:HB1	2.27	0.48
1:B:764:MET:CE	1:B:770:TYR:CE2	2.96	0.48
1:B:782:LYS:HA	1:B:785:GLU:OE1	2.13	0.48
1:B:891:GLU:O	1:B:894:LYS:HB2	2.13	0.48
1:C:716:THR:HG23	1:C:923:LYS:CD	2.41	0.48
1:C:793:LYS:HB3	1:C:892:LEU:HD12	1.95	0.48
1:A:816:VAL:HA	1:B:636:VAL:HG21	1.94	0.48
1:B:652:TYR:CD2	1:B:683:LYS:HD2	2.49	0.48
1:B:654:ARG:O	1:B:656:GLN:N	2.46	0.48
1:A:711:LYS:HG2	1:A:767:ILE:HD11	1.95	0.48
1:A:864:VAL:CG1	1:A:865:GLU:N	2.76	0.48
1:D:680:LEU:O	1:D:681:LYS:HB3	2.14	0.48
1:D:762:PHE:O	1:D:766:ARG:HG2	2.13	0.48
1:D:939:PHE:CE2	1:D:943:GLU:OE1	2.66	0.48
1:A:923:LYS:O	1:A:923:LYS:HG2	2.13	0.48
1:C:856:LEU:HA	1:D:649:PHE:CZ	2.48	0.48
1:D:681:LYS:C	1:D:682:VAL:HG22	2.34	0.48
1:A:967:ILE:HD11	1:A:971:GLU:CD	2.34	0.48
1:A:815:GLU:O	1:A:818:LEU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:LEU:HD23	1:C:686:SER:N	2.29	0.48
1:C:892:LEU:O	1:C:892:LEU:HD23	2.13	0.48
1:C:714:ILE:HD13	1:C:770:TYR:CE2	2.49	0.48
1:C:837:ILE:HG13	1:C:838:SER:N	2.29	0.48
1:D:883:GLN:HE21	1:D:886:LYS:NZ	2.12	0.48
1:D:919:GLN:HB3	1:D:920:PRO:HD2	1.96	0.48
1:B:867:LYS:HE2	2:B:42:HOH:O	2.14	0.48
1:C:867:LYS:CD	1:D:639:ILE:HG22	2.40	0.48
1:B:1001:GLU:O	1:B:1005:ARG:HG3	2.14	0.47
1:C:752:ASP:HA	1:C:759:ARG:HH12	1.79	0.47
1:C:789:GLU:O	1:C:793:LYS:HD2	2.14	0.47
1:D:751:LEU:HD23	1:D:751:LEU:N	2.28	0.47
1:D:897:SER:CA	1:D:900:ARG:HG2	2.37	0.47
1:A:899:LEU:O	1:A:903:LEU:HB2	2.15	0.47
1:A:896:ILE:HG13	1:A:946:LEU:HD22	1.94	0.47
1:C:615:TRP:CD1	1:C:615:TRP:N	2.76	0.47
1:C:809:ALA:HB3	1:C:874:LEU:CD1	2.42	0.47
1:D:882:PRO:HA	1:D:977:ASP:OD1	2.14	0.47
1:A:829:ARG:HD2	1:B:739:SER:OG	2.15	0.47
1:B:755:ALA:HB3	1:B:758:ASP:OD2	2.14	0.47
1:B:828:GLN:O	1:B:829:ARG:NH2	2.48	0.47
1:C:727:MET:HA	1:C:727:MET:CE	2.44	0.47
1:C:786:ARG:NH1	1:C:898:THR:HG22	2.25	0.47
1:D:797:ILE:HD11	1:D:887:VAL:HG11	1.95	0.47
1:D:902:GLY:O	1:D:906:VAL:HG23	2.15	0.47
1:B:601:LYS:O	1:B:603:ILE:HG13	2.15	0.47
1:A:833:TYR:HB2	1:B:623:LEU:HD21	1.93	0.47
1:D:813:LEU:HD23	1:D:871:VAL:HG11	1.96	0.47
1:D:994:ARG:NH2	1:D:995:LYS:HE3	2.29	0.47
1:A:630:GLU:HB2	1:B:811:LYS:NZ	2.29	0.47
1:A:996:LYS:O	1:A:1000:GLU:HG2	2.14	0.47
1:C:624:GLU:CD	1:C:625:GLY:N	2.68	0.47
1:C:735:VAL:HG12	1:C:770:TYR:HE1	1.79	0.47
1:C:836:LYS:N	1:D:618:LEU:HD13	2.30	0.47
1:C:839:SER:OG	1:D:615:TRP:HA	2.14	0.47
1:C:865:GLU:O	1:C:869:PRO:HG3	2.14	0.47
1:C:637:PHE:HE2	1:D:823:TYR:HB2	1.78	0.47
1:D:900:ARG:NH1	1:D:943:GLU:OE2	2.47	0.47
1:A:967:ILE:O	1:A:967:ILE:HG23	2.13	0.47
1:C:621:ASN:C	1:C:623:LEU:H	2.18	0.47
1:C:812:GLN:O	1:C:816:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:LEU:HD22	1:C:881:ILE:HD12	1.96	0.47
1:B:613:PHE:O	1:B:614:ASN:CB	2.62	0.47
1:B:655:GLN:HG2	1:B:753:ARG:HH21	1.79	0.47
1:B:862:THR:HG23	1:B:990:ASN:HD22	1.77	0.47
1:B:888:ASN:HD22	1:B:891:GLU:HB2	1.78	0.47
1:C:769:HIS:HB3	1:C:772:GLN:HG3	1.97	0.47
1:C:843:ILE:HG12	1:D:613:PHE:CE1	2.50	0.47
1:D:896:ILE:HG13	1:D:946:LEU:HD22	1.95	0.47
1:A:642:LEU:O	1:A:646:GLU:HG3	2.15	0.47
1:A:953:PHE:O	1:A:957:VAL:HG23	2.14	0.47
1:A:849:SER:O	1:B:653:GLN:OE1	2.33	0.47
1:B:910:LEU:CD2	1:B:932:ILE:HD12	2.44	0.47
1:D:714:ILE:C	1:D:714:ILE:HD12	2.34	0.47
1:D:764:MET:HE2	1:D:770:TYR:HE2	1.80	0.47
1:C:728:LEU:CD2	1:C:777:LEU:HG	2.41	0.47
1:C:772:GLN:HB2	1:C:909:GLU:HG2	1.97	0.47
1:A:613:PHE:HE1	1:B:843:ILE:HA	1.80	0.46
1:B:621:ASN:ND2	1:B:622:LYS:HG3	2.29	0.46
1:C:745:GLU:CD	1:C:766:ARG:HH12	2.19	0.46
1:A:837:ILE:HG13	1:A:838:SER:N	2.30	0.46
1:A:963:GLU:O	1:A:964:ALA:O	2.33	0.46
1:C:630:GLU:HB2	1:D:811:LYS:HE2	1.97	0.46
1:C:838:SER:HA	1:C:975:ILE:CG2	2.45	0.46
1:D:608:ASN:HB3	2:D:68:HOH:O	2.15	0.46
1:A:613:PHE:O	1:A:614:ASN:HB3	2.15	0.46
1:B:655:GLN:O	1:B:657:ASP:N	2.48	0.46
1:C:613:PHE:O	1:C:614:ASN:HB3	2.15	0.46
1:C:751:LEU:O	1:C:759:ARG:NH1	2.49	0.46
1:C:900:ARG:HG3	1:C:901:SER:H	1.81	0.46
1:C:811:LYS:HE3	1:D:627:VAL:HG12	1.98	0.46
1:D:685:LEU:C	1:D:685:LEU:HD23	2.36	0.46
1:D:883:GLN:NE2	1:D:886:LYS:HZ1	2.14	0.46
1:B:613:PHE:CD1	1:B:613:PHE:C	2.84	0.46
1:C:711:LYS:CG	1:C:767:ILE:HD11	2.39	0.46
1:C:797:ILE:HD11	1:C:969:PRO:HG2	1.97	0.46
1:C:997:LYS:HZ2	1:C:998:GLU:HG2	1.81	0.46
1:C:623:LEU:CD2	1:D:833:TYR:HB3	2.39	0.46
1:B:610:LEU:CD2	1:B:646:GLU:HA	2.44	0.46
1:C:748:LYS:HE3	1:C:748:LYS:HB2	1.69	0.46
1:C:741:ILE:CG1	1:C:765:SER:HB2	2.46	0.46
1:D:750:GLU:C	1:D:752:ASP:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:824:MET:HE3	1:D:856:LEU:HD22	1.98	0.46
1:A:621:ASN:C	1:A:623:LEU:H	2.19	0.46
1:B:745:GLU:O	1:B:747:HIS:N	2.49	0.46
1:B:795:GLU:OE2	1:B:798:ARG:NH2	2.37	0.46
1:C:619:PRO:HB2	1:C:622:LYS:HD3	1.96	0.46
1:C:769:HIS:HB3	1:C:772:GLN:HG2	1.97	0.46
1:C:897:SER:O	1:C:900:ARG:HG3	2.16	0.46
1:C:910:LEU:HD23	1:C:932:ILE:HD12	1.97	0.46
1:D:892:LEU:C	1:D:892:LEU:HD23	2.36	0.46
1:A:868:TYR:OH	1:B:639:ILE:HD12	2.15	0.46
1:B:745:GLU:C	1:B:747:HIS:H	2.18	0.46
1:C:741:ILE:HD11	1:C:765:SER:HB2	1.97	0.46
1:C:958:LYS:O	1:C:958:LYS:HG2	2.15	0.46
1:A:864:VAL:HG13	1:A:865:GLU:N	2.29	0.46
1:A:939:PHE:C	1:A:941:ASP:N	2.67	0.46
1:B:860:LEU:O	1:B:864:VAL:HB	2.16	0.46
1:D:869:PRO:O	1:D:872:LEU:HB2	2.16	0.46
1:A:692:ARG:HH22	1:A:740:ASP:CG	2.20	0.46
1:B:716:THR:CG2	1:B:923:LYS:HE3	2.46	0.46
1:C:614:ASN:O	1:C:614:ASN:CG	2.53	0.46
1:A:753:ARG:HA	1:A:753:ARG:NH1	2.30	0.45
1:A:815:GLU:HG3	1:B:631:ILE:HG23	1.98	0.45
1:A:860:LEU:O	1:A:864:VAL:HB	2.15	0.45
1:A:963:GLU:O	1:A:964:ALA:C	2.54	0.45
1:D:844:ALA:HA	1:D:855:THR:OG1	2.16	0.45
1:D:859:TYR:O	1:D:863:ILE:HG23	2.16	0.45
1:D:883:GLN:HE21	1:D:886:LYS:HZ1	1.64	0.45
1:B:837:ILE:O	1:B:840:LEU:HB2	2.16	0.45
1:B:864:VAL:HG11	1:B:871:VAL:HG11	1.99	0.45
1:B:600:LYS:HG2	1:B:601:LYS:N	2.31	0.45
1:B:885:ALA:O	1:B:970:ASP:HA	2.15	0.45
1:C:710:ILE:HG21	1:C:764:MET:HE1	1.98	0.45
1:A:710:ILE:O	1:A:711:LYS:C	2.52	0.45
1:A:939:PHE:O	1:A:940:SER:C	2.54	0.45
1:D:1002:ARG:O	1:D:1003:ARG:C	2.54	0.45
1:D:687:VAL:HG21	1:D:743:LEU:HD22	1.98	0.45
1:D:689:ASP:OD1	1:D:692:ARG:HB2	2.15	0.45
1:D:786:ARG:HA	1:D:789:GLU:OE1	2.17	0.45
1:A:652:TYR:HE2	1:A:750:GLU:OE2	2.00	0.45
1:B:716:THR:HG23	1:B:923:LYS:HE3	1.99	0.45
1:B:804:VAL:HG22	1:B:881:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:MET:O	1:A:755:ALA:C	2.55	0.45
1:C:641:ASP:OD1	1:C:644:ASP:HB2	2.17	0.45
1:C:753:ARG:HA	1:C:753:ARG:NE	2.32	0.45
1:A:888:ASN:HD22	1:A:891:GLU:HB2	1.82	0.45
1:B:764:MET:CE	1:B:770:TYR:HE2	2.30	0.45
1:C:695:ASN:N	1:C:695:ASN:ND2	2.64	0.45
1:C:833:TYR:HB3	1:D:623:LEU:HD21	1.97	0.45
1:A:818:LEU:HD23	1:B:633:ASP:HB3	1.98	0.45
1:B:981:GLN:O	1:B:984:SER:N	2.50	0.45
1:C:613:PHE:HD1	1:C:613:PHE:C	2.19	0.45
1:C:622:LYS:H	1:C:622:LYS:HD2	1.81	0.45
1:C:735:VAL:HG12	1:C:770:TYR:CE1	2.52	0.45
1:C:788:ALA:O	1:C:792:PRO:HD2	2.17	0.45
1:D:889:MET:HE3	1:D:892:LEU:HB3	1.99	0.45
1:A:867:LYS:HE3	1:B:639:ILE:O	2.17	0.44
1:B:751:LEU:CG	1:B:759:ARG:HH12	2.29	0.44
1:B:824:MET:O	1:B:826:LYS:N	2.49	0.44
1:D:687:VAL:HG23	1:D:688:ILE:N	2.32	0.44
1:A:606:PRO:HG3	1:B:823:TYR:CE1	2.53	0.44
1:A:783:PHE:O	1:A:787:VAL:HG12	2.17	0.44
1:C:791:LYS:HA	1:C:794:VAL:HG12	1.99	0.44
1:C:606:PRO:HB3	1:D:823:TYR:CE2	2.52	0.44
1:D:862:THR:HG22	1:D:863:ILE:N	2.33	0.44
1:D:897:SER:HA	1:D:900:ARG:CG	2.39	0.44
1:D:985:GLU:O	1:D:988:GLN:HG2	2.17	0.44
1:A:849:SER:HB2	1:B:653:GLN:HE21	1.75	0.44
1:B:769:HIS:O	1:B:773:ARG:HG3	2.17	0.44
1:B:828:GLN:HG2	1:B:829:ARG:HH22	1.82	0.44
1:B:996:LYS:O	1:B:1000:GLU:CG	2.65	0.44
1:C:745:GLU:C	1:C:747:HIS:H	2.21	0.44
1:A:769:HIS:HB3	1:A:772:GLN:CG	2.47	0.44
1:B:762:PHE:O	1:B:766:ARG:HG2	2.18	0.44
1:C:716:THR:HG22	1:C:719:GLU:HB3	1.99	0.44
1:C:861:ILE:O	1:C:865:GLU:HG3	2.17	0.44
1:D:963:GLU:O	1:D:964:ALA:C	2.56	0.44
1:A:652:TYR:CE2	1:A:750:GLU:OE2	2.71	0.44
1:A:724:PRO:HG2	1:A:727:MET:HG2	2.00	0.44
1:B:643:GLU:OE2	1:B:647:ARG:NE	2.45	0.44
1:B:769:HIS:CD2	1:B:772:GLN:HG3	2.53	0.44
1:C:820:PHE:HB3	1:C:824:MET:HE3	1.99	0.44
1:A:991:GLU:O	1:A:995:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:VAL:HG23	1:B:815:GLU:HG2	2.00	0.44
1:B:829:ARG:NE	1:B:829:ARG:CA	2.73	0.44
1:C:864:VAL:HG13	1:C:865:GLU:N	2.31	0.44
1:D:682:VAL:O	1:D:683:LYS:CD	2.66	0.44
1:D:769:HIS:HD2	1:D:909:GLU:OE1	2.01	0.44
1:D:791:LYS:O	1:D:794:VAL:CG1	2.66	0.44
1:D:812:GLN:HE21	1:D:816:VAL:HG23	1.83	0.44
1:A:986:ALA:O	1:A:990:ASN:HB2	2.18	0.44
1:B:652:TYR:HD2	1:B:683:LYS:HD2	1.83	0.44
1:C:681:LYS:HZ1	1:C:683:LYS:HD3	1.82	0.44
1:C:812:GLN:NE2	1:C:868:TYR:CE2	2.86	0.44
1:A:843:ILE:HG12	1:B:613:PHE:CE1	2.53	0.44
1:B:603:ILE:HG22	1:B:605:GLN:HG3	2.00	0.44
1:C:716:THR:HG22	1:C:716:THR:O	2.18	0.44
1:C:839:SER:OG	1:D:615:TRP:CB	2.66	0.44
1:B:652:TYR:HA	1:B:684:GLU:O	2.18	0.43
1:B:751:LEU:HB2	1:B:759:ARG:HH11	1.83	0.43
1:B:769:HIS:O	1:B:773:ARG:HG2	2.18	0.43
1:C:630:GLU:OE1	1:D:811:LYS:HE3	2.17	0.43
1:C:924:PHE:CD1	1:C:928:VAL:HG21	2.52	0.43
1:D:792:PRO:HG2	1:D:793:LYS:H	1.82	0.43
1:A:641:ASP:OD1	1:A:641:ASP:O	2.36	0.43
1:B:730:GLN:HE22	1:B:733:LYS:HE3	1.82	0.43
1:B:836:LYS:HB3	1:B:836:LYS:HE2	1.78	0.43
1:D:728:LEU:HD21	1:D:777:LEU:HG	2.00	0.43
1:A:1000:GLU:HA	1:A:1000:GLU:OE1	2.19	0.43
1:A:907:GLU:HA	1:A:932:ILE:CD1	2.48	0.43
1:B:751:LEU:CD1	1:B:759:ARG:HH12	2.31	0.43
1:D:689:ASP:OD2	1:D:691:ARG:HB3	2.18	0.43
1:D:754:MET:O	1:D:755:ALA:C	2.57	0.43
1:B:907:GLU:HA	1:B:932:ILE:HD11	2.01	0.43
1:D:680:LEU:O	1:D:681:LYS:CB	2.67	0.43
1:D:840:LEU:C	1:D:842:LYS:H	2.21	0.43
1:D:864:VAL:HG13	1:D:865:GLU:N	2.32	0.43
1:A:809:ALA:CB	1:A:877:GLU:OE2	2.67	0.43
1:D:706:SER:O	1:D:710:ILE:HG13	2.18	0.43
1:D:802:GLU:HG3	1:D:806:ARG:HD2	2.00	0.43
1:A:772:GLN:CA	1:A:772:GLN:HE21	2.31	0.43
1:A:610:LEU:HD12	1:B:824:MET:HA	2.01	0.43
1:B:922:ASP:C	1:B:922:ASP:OD1	2.57	0.43
1:C:788:ALA:O	1:C:792:PRO:CD	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:997:LYS:HD3	1:C:998:GLU:CA	2.47	0.43
1:C:820:PHE:CE1	1:D:640:LEU:HD11	2.54	0.43
1:D:764:MET:HE2	1:D:770:TYR:CE2	2.53	0.43
1:A:745:GLU:C	1:A:747:HIS:H	2.22	0.43
1:C:728:LEU:HD23	1:C:778:TYR:HA	2.00	0.43
1:D:749:HIS:O	1:D:750:GLU:OE1	2.36	0.43
1:A:837:ILE:CG2	1:A:960:PHE:HD2	2.32	0.43
1:A:967:ILE:CD1	1:A:971:GLU:CD	2.87	0.43
1:A:999:GLU:CG	1:A:1003:ARG:HG3	2.49	0.43
1:C:621:ASN:ND2	1:C:622:LYS:HZ2	2.16	0.43
1:C:790:VAL:O	1:C:793:LYS:HB2	2.19	0.43
1:C:838:SER:HA	1:C:975:ILE:HG21	2.00	0.43
1:C:879:ARG:HH11	1:C:879:ARG:HG3	1.84	0.43
1:B:634:THR:HG22	1:B:635:LYS:N	2.33	0.43
1:B:716:THR:HG21	1:B:719:GLU:HG2	2.00	0.43
1:C:815:GLU:OE1	1:D:631:ILE:HA	2.19	0.43
1:A:739:SER:HB2	1:B:829:ARG:HD3	2.01	0.42
1:C:791:LYS:O	1:C:794:VAL:CG1	2.62	0.42
1:C:888:ASN:HB2	2:C:66:HOH:O	2.17	0.42
1:D:724:PRO:HG2	1:D:727:MET:HG3	2.00	0.42
1:D:896:ILE:HG13	1:D:946:LEU:CD2	2.48	0.42
1:A:918:PRO:O	1:A:919:GLN:CG	2.68	0.42
1:B:787:VAL:HG13	1:B:788:ALA:N	2.33	0.42
1:A:642:LEU:HD13	1:B:823:TYR:CZ	2.54	0.42
1:C:710:ILE:CG2	1:C:764:MET:HE1	2.49	0.42
1:D:917:PRO:HA	1:D:918:PRO:HD3	1.95	0.42
1:B:749:HIS:N	1:B:749:HIS:ND1	2.62	0.42
1:B:967:ILE:HD11	1:B:972:PHE:HA	2.01	0.42
1:B:971:GLU:O	1:B:975:ILE:HG13	2.19	0.42
1:C:999:GLU:OE1	1:C:1000:GLU:HA	2.19	0.42
1:D:759:ARG:O	1:D:763:GLU:HG2	2.20	0.42
1:D:813:LEU:C	1:D:813:LEU:HD13	2.40	0.42
1:A:751:LEU:HG	1:A:759:ARG:NH1	2.34	0.42
1:B:613:PHE:CD1	1:B:613:PHE:O	2.73	0.42
1:B:653:GLN:HB2	1:B:656:GLN:NE2	2.34	0.42
1:B:657:ASP:O	1:B:658:PHE:O	2.37	0.42
1:C:864:VAL:CG1	1:C:865:GLU:N	2.82	0.42
1:C:858:HIS:HB3	1:C:990:ASN:OD1	2.19	0.42
1:D:900:ARG:HH12	1:D:943:GLU:CD	2.23	0.42
1:A:957:VAL:HG13	1:A:962:GLU:HB2	2.01	0.42
1:C:1000:GLU:OE1	1:C:1001:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:772:GLN:CD	1:C:772:GLN:H	2.23	0.42
1:C:855:THR:HG1	1:C:858:HIS:CE1	2.31	0.42
1:D:608:ASN:CB	2:D:68:HOH:O	2.66	0.42
1:D:724:PRO:HG2	1:D:727:MET:CG	2.49	0.42
1:A:769:HIS:CE1	1:A:912:TYR:CZ	3.08	0.42
1:B:924:PHE:CE1	1:B:928:VAL:HG21	2.54	0.42
1:C:635:LYS:CB	1:C:635:LYS:NZ	2.82	0.42
1:C:820:PHE:CE2	1:C:860:LEU:HD23	2.55	0.42
1:C:881:ILE:N	1:C:882:PRO:CD	2.83	0.42
1:D:748:LYS:O	1:D:751:LEU:HD22	2.19	0.42
1:D:773:ARG:NH2	1:D:913:GLN:NE2	2.68	0.42
1:D:900:ARG:HH11	1:D:900:ARG:HB3	1.82	0.42
1:A:601:LYS:O	1:A:603:ILE:CG1	2.67	0.42
1:B:614:ASN:ND2	1:B:614:ASN:O	2.52	0.42
1:A:636:VAL:HG21	1:B:816:VAL:HA	2.01	0.42
1:B:873:ASN:N	1:B:873:ASN:OD1	2.52	0.42
1:B:907:GLU:CG	1:B:932:ILE:HD13	2.50	0.42
1:C:798:ARG:HG2	1:C:798:ARG:HH11	1.85	0.42
1:C:824:MET:HE1	1:D:645:LEU:HD11	2.01	0.42
1:A:699:LEU:HD13	1:A:730:GLN:HB3	2.00	0.42
1:B:699:LEU:C	1:B:699:LEU:HD12	2.39	0.42
1:B:903:LEU:HD23	1:B:903:LEU:HA	1.84	0.42
1:B:918:PRO:O	1:B:919:GLN:CG	2.67	0.42
1:D:826:LYS:HE3	1:D:826:LYS:C	2.39	0.42
1:B:838:SER:O	1:B:839:SER:C	2.57	0.42
1:C:803:GLU:HB3	1:C:877:GLU:O	2.19	0.42
1:C:639:ILE:HG22	1:D:867:LYS:HD3	2.02	0.42
1:A:901:SER:O	1:A:904:LYS:HB2	2.19	0.42
1:C:785:GLU:HB2	2:C:15:HOH:O	2.19	0.42
1:C:794:VAL:CG1	1:C:795:GLU:N	2.82	0.42
1:D:703:LEU:C	1:D:703:LEU:HD23	2.40	0.42
1:A:623:LEU:HD12	1:A:623:LEU:HA	1.90	0.41
1:B:837:ILE:H	1:B:837:ILE:HG13	1.58	0.41
1:C:907:GLU:HA	1:C:932:ILE:CD1	2.43	0.41
1:B:782:LYS:O	1:B:786:ARG:HD2	2.20	0.41
1:C:612:SER:HB3	1:C:743:LEU:CD1	2.51	0.41
1:D:820:PHE:O	1:D:824:MET:HG2	2.20	0.41
1:D:988:GLN:CG	1:D:989:GLU:N	2.83	0.41
1:B:768:ASN:O	1:B:773:ARG:NE	2.47	0.41
1:C:889:MET:HA	1:C:889:MET:CE	2.50	0.41
1:C:631:ILE:HG23	1:D:815:GLU:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:785:GLU:N	2:C:15:HOH:O	2.53	0.41
1:C:876:GLU:OE1	1:C:876:GLU:N	2.52	0.41
1:D:828:GLN:NE2	1:D:829:ARG:NH2	2.64	0.41
1:D:900:ARG:NH1	1:D:900:ARG:CB	2.83	0.41
1:A:688:ILE:HB	1:A:758:ASP:OD1	2.20	0.41
1:A:820:PHE:O	1:A:824:MET:HG2	2.21	0.41
1:B:907:GLU:HA	1:B:932:ILE:CD1	2.51	0.41
1:B:925:VAL:HB	2:B:30:HOH:O	2.20	0.41
1:C:633:ASP:N	1:C:633:ASP:OD1	2.53	0.41
1:D:941:ASP:O	1:D:944:ASP:HB2	2.20	0.41
1:B:809:ALA:O	1:B:813:LEU:HB2	2.21	0.41
1:C:845:ASP:HB3	1:D:689:ASP:OD2	2.20	0.41
1:D:858:HIS:ND1	1:D:986:ALA:HB1	2.36	0.41
1:B:855:THR:HG23	1:B:857:LEU:N	2.34	0.41
1:C:635:LYS:HZ2	1:C:635:LYS:CB	2.33	0.41
1:C:695:ASN:H	1:C:695:ASN:ND2	2.19	0.41
1:C:875:ASN:HB2	1:C:876:GLU:OE1	2.20	0.41
1:D:614:ASN:CG	1:D:614:ASN:O	2.58	0.41
1:A:909:GLU:OE2	1:A:913:GLN:HG2	2.21	0.41
1:C:611:LYS:HE3	1:C:650:SER:O	2.21	0.41
1:C:858:HIS:HA	1:C:990:ASN:HD21	1.85	0.41
1:C:992:ASN:O	1:C:995:LYS:HE3	2.21	0.41
1:D:820:PHE:O	1:D:824:MET:CG	2.69	0.41
1:D:889:MET:CE	1:D:889:MET:HA	2.51	0.41
1:D:932:ILE:O	1:D:936:SER:HB2	2.21	0.41
1:A:754:MET:O	1:A:755:ALA:O	2.38	0.41
1:A:756:LYS:HE3	1:A:756:LYS:HB2	1.86	0.41
1:B:718:ASP:OD1	1:B:721:GLU:N	2.54	0.41
1:B:855:THR:O	1:B:858:HIS:N	2.54	0.41
1:C:835:PHE:CD1	1:C:835:PHE:C	2.94	0.41
1:C:910:LEU:HD11	1:C:925:VAL:HG13	2.03	0.41
1:C:992:ASN:HA	1:C:995:LYS:CD	2.50	0.41
1:B:615:TRP:N	1:B:615:TRP:CD1	2.83	0.41
1:B:867:LYS:O	1:B:868:TYR:CG	2.74	0.41
1:C:885:ALA:O	1:C:970:ASP:HA	2.20	0.41
1:D:717:MET:CE	1:D:717:MET:HA	2.51	0.41
1:D:851:ASP:HA	2:D:69:HOH:O	2.21	0.41
1:A:652:TYR:N	1:A:652:TYR:CD1	2.89	0.41
1:C:723:LEU:CB	1:C:728:LEU:HD11	2.45	0.41
1:D:603:ILE:HA	1:D:604:PRO:HD3	1.91	0.41
1:C:833:TYR:CB	1:D:623:LEU:HD21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:GLU:C	1:A:747:HIS:N	2.74	0.40
1:B:746:GLU:H	1:B:746:GLU:CD	2.24	0.40
1:B:868:TYR:N	1:B:869:PRO:CD	2.82	0.40
1:D:739:SER:O	1:D:743:LEU:HB2	2.21	0.40
1:A:1004:ALA:O	1:A:1008:ALA:CB	2.69	0.40
1:C:820:PHE:HB3	1:C:824:MET:CE	2.50	0.40
1:C:649:PHE:CE2	1:D:848:SER:HA	2.56	0.40
1:A:615:TRP:N	1:A:615:TRP:CD1	2.88	0.40
1:A:836:LYS:HB3	1:A:836:LYS:HE2	1.97	0.40
1:A:981:GLN:O	1:A:984:SER:N	2.55	0.40
1:B:826:LYS:HG3	1:B:827:GLY:N	2.36	0.40
1:A:923:LYS:HG2	1:A:926:SER:HB3	2.04	0.40
1:A:837:ILE:HG13	1:A:975:ILE:HD13	2.02	0.40
1:B:896:ILE:HA	1:B:896:ILE:HD13	1.93	0.40
1:C:653:GLN:HE21	1:D:849:SER:HA	1.86	0.40
1:D:888:ASN:HD22	1:D:891:GLU:H	1.66	0.40
1:B:723:LEU:HB3	1:B:728:LEU:CD1	2.29	0.40
1:B:741:ILE:HG12	1:B:765:SER:HB2	2.03	0.40
1:C:999:GLU:C	1:C:999:GLU:OE1	2.60	0.40
1:D:753:ARG:CA	1:D:753:ARG:HE	2.27	0.40
1:D:764:MET:CE	1:D:770:TYR:HE2	2.33	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	384/419 (92%)	330 (86%)	46 (12%)	8 (2%)	7 23
1	B	392/419 (94%)	329 (84%)	51 (13%)	12 (3%)	4 14
1	C	375/419 (90%)	312 (83%)	53 (14%)	10 (3%)	5 17
1	D	386/419 (92%)	331 (86%)	44 (11%)	11 (3%)	5 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1537/1676 (92%)	1302 (85%)	194 (13%)	41 (3%)	5 17

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	755	ALA
1	A	824	MET
1	A	964	ALA
1	B	655	GLN
1	B	658	PHE
1	B	746	GLU
1	B	824	MET
1	B	964	ALA
1	C	965	GLY
1	D	681	LYS
1	D	682	VAL
1	D	824	MET
1	D	964	ALA
1	B	614	ASN
1	B	656	GLN
1	C	964	ALA
1	D	655	GLN
1	D	746	GLU
1	D	982	ALA
1	A	825	ASN
1	A	982	ALA
1	B	825	ASN
1	C	824	MET
1	C	982	ALA
1	D	755	ALA
1	A	753	ARG
1	A	890	THR
1	B	753	ARG
1	C	614	ASN
1	C	622	LYS
1	C	884	ALA
1	C	924	PHE
1	D	753	ARG
1	D	841	ASN
1	A	614	ASN
1	B	601	LYS
1	B	628	TRP

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Mol	Chain	Res	Type
1	B	890	THR
1	C	736	PRO
1	D	873	ASN
1	C	628	TRP

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	350/377 (93%)	315 (90%)	35 (10%)	7 22
1	B	356/377 (94%)	319 (90%)	37 (10%)	7 21
1	C	343/377 (91%)	311 (91%)	32 (9%)	9 26
1	D	352/377 (93%)	315 (90%)	37 (10%)	7 20
All	All	1401/1508 (93%)	1260 (90%)	141 (10%)	7 22

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	615	TRP
1	A	621	ASN
1	A	624	GLU
1	A	627	VAL
1	A	639	ILE
1	A	701	SER
1	A	714	ILE
1	A	728	LEU
1	A	751	LEU
1	A	753	ARG
1	A	772	GLN
1	A	774	LEU
1	A	780	LYS
1	A	789	GLU
1	A	794	VAL
1	A	798	ARG
1	A	799	SER

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Mol	Chain	Res	Type
1	A	814	LEU
1	A	825	ASN
1	A	829	ARG
1	A	857	LEU
1	A	860	LEU
1	A	863	ILE
1	A	866	ASN
1	A	872	LEU
1	A	879	ARG
1	A	883	GLN
1	A	895	GLU
1	A	903	LEU
1	A	941	ASP
1	A	943	GLU
1	A	952	LEU
1	A	970	ASP
1	A	985	GLU
1	A	993	MET
1	B	598	LEU
1	B	601	LYS
1	B	615	TRP
1	B	627	VAL
1	B	634	THR
1	B	643	GLU
1	B	659	PHE
1	B	703	LEU
1	B	708	ASP
1	B	714	ILE
1	B	716	THR
1	B	723	LEU
1	B	731	LEU
1	B	737	GLU
1	B	748	LYS
1	B	749	HIS
1	B	751	LEU
1	B	769	HIS
1	B	771	GLN
1	B	772	GLN
1	B	774	LEU
1	B	775	GLN
1	B	780	LYS
1	B	813	LEU

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Mol	Chain	Res	Type
1	B	825	ASN
1	B	837	ILE
1	B	855	THR
1	B	857	LEU
1	B	860	LEU
1	B	862	THR
1	B	863	ILE
1	B	864	VAL
1	B	873	ASN
1	B	880	ASP
1	B	897	SER
1	B	909	GLU
1	B	966	LYS
1	C	613	PHE
1	C	615	TRP
1	C	621	ASN
1	C	624	GLU
1	C	627	VAL
1	C	643	GLU
1	C	685	LEU
1	C	702	ARG
1	C	719	GLU
1	C	743	LEU
1	C	752	ASP
1	C	753	ARG
1	C	758	ASP
1	C	771	GLN
1	C	772	GLN
1	C	774	LEU
1	C	825	ASN
1	C	829	ARG
1	C	835	PHE
1	C	860	LEU
1	C	889	MET
1	C	890	THR
1	C	893	ASP
1	C	903	LEU
1	C	938	SER
1	C	941	ASP
1	C	970	ASP
1	C	995	LYS
1	C	996	LYS

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Mol	Chain	Res	Type
1	C	999	GLU
1	C	1000	GLU
1	C	1002	ARG
1	D	615	TRP
1	D	627	VAL
1	D	643	GLU
1	D	654	ARG
1	D	682	VAL
1	D	716	THR
1	D	728	LEU
1	D	731	LEU
1	D	743	LEU
1	D	749	HIS
1	D	751	LEU
1	D	769	HIS
1	D	772	GLN
1	D	774	LEU
1	D	775	GLN
1	D	782	LYS
1	D	814	LEU
1	D	825	ASN
1	D	826	LYS
1	D	828	GLN
1	D	829	ARG
1	D	836	LYS
1	D	847	LYS
1	D	857	LEU
1	D	863	ILE
1	D	872	LEU
1	D	900	ARG
1	D	903	LEU
1	D	916	GLN
1	D	932	ILE
1	D	952	LEU
1	D	954	THR
1	D	958	LYS
1	D	984	SER
1	D	990	ASN
1	D	997	LYS
1	D	1005	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	653	GLN
1	A	768	ASN
1	A	769	HIS
1	A	771	GLN
1	A	772	GLN
1	A	775	GLN
1	A	828	GLN
1	A	853	ASN
1	A	858	HIS
1	A	866	ASN
1	A	888	ASN
1	A	913	GLN
1	A	968	GLN
1	A	1009	GLN
1	B	614	ASN
1	B	653	GLN
1	B	655	GLN
1	B	656	GLN
1	B	695	ASN
1	B	730	GLN
1	B	768	ASN
1	B	769	HIS
1	B	772	GLN
1	B	812	GLN
1	B	828	GLN
1	B	853	ASN
1	B	858	HIS
1	B	866	ASN
1	B	888	ASN
1	C	621	ASN
1	C	653	GLN
1	C	655	GLN
1	C	695	ASN
1	C	697	ASN
1	C	768	ASN
1	C	769	HIS
1	C	812	GLN
1	C	828	GLN
1	C	888	ASN
1	C	913	GLN
1	C	930	GLN
1	C	978	GLN
1	C	992	ASN

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Mol	Chain	Res	Type
1	D	614	ASN
1	D	653	GLN
1	D	768	ASN
1	D	769	HIS
1	D	772	GLN
1	D	812	GLN
1	D	828	GLN
1	D	858	HIS
1	D	866	ASN
1	D	883	GLN
1	D	888	ASN
1	D	913	GLN
1	D	968	GLN
1	D	988	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	388/419 (92%)	-0.08	4 (1%)	82	77	24, 60, 116, 152	0
1	B	396/419 (94%)	-0.11	4 (1%)	82	77	30, 62, 107, 141	0
1	C	379/419 (90%)	0.08	19 (5%)	28	19	36, 78, 131, 162	0
1	D	390/419 (93%)	-0.08	6 (1%)	73	68	36, 67, 115, 155	0
All	All	1553/1676 (92%)	-0.05	33 (2%)	63	54	24, 66, 119, 162	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	680	LEU	5.8
1	C	929	SER	5.1
1	C	714	ILE	4.5
1	C	656	GLN	4.0
1	C	1001	GLU	3.8
1	C	928	VAL	3.7
1	C	921	GLY	3.2
1	A	1010	LEU	3.1
1	C	935	ALA	3.1
1	C	932	ILE	2.9
1	A	1002	ARG	2.9
1	C	925	VAL	2.8
1	C	1000	GLU	2.8
1	B	653	GLN	2.8
1	C	939	PHE	2.7
1	D	714	ILE	2.7
1	A	998	GLU	2.7
1	B	1010	LEU	2.6
1	D	642	LEU	2.6
1	C	920	PRO	2.5
1	C	998	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1007	GLU	2.3
1	C	993	MET	2.3
1	D	650	SER	2.3
1	D	681	LYS	2.3
1	B	656	GLN	2.2
1	C	850	ILE	2.2
1	C	997	LYS	2.2
1	C	924	PHE	2.2
1	C	931	PHE	2.2
1	B	625	GLY	2.1
1	C	717	MET	2.1
1	D	657	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 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.