Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 02:11 AM EDT

PDB ID	:	3SDM
Title	:	Structure of oligomeric kinase/RNase Ire1 in complex with an oligonucleotide
Authors	:	Korennykh, A.; Korostelev, A.; Egea, P.; Finer-Moore, J.; Zhang, C.; Stroud, R.; Shokat, K.; Walter, P.
Deposited on	:	2011-06-09
Resolution	:	6.60 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

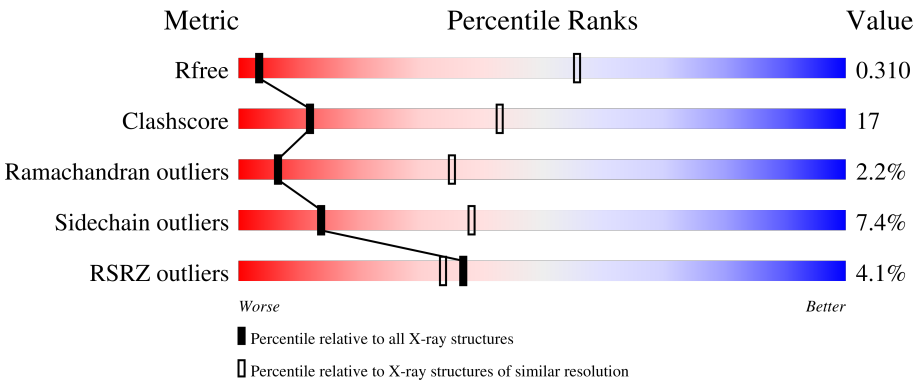
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 6.60 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	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)
RSRZ outliers	127900	1002 (9.00-3.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	448	9% 57% 31% 5% 7%
1	B	448	4% 58% 30% 5% 7%
1	C	448	4% 58% 29% 5% 7%
1	D	448	4% 58% 29% 6% 7%
1	E	448	2% 57% 31% 5% 7%

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Mol	Chain	Length	Quality of chain
1	F	448	% 57% 31% 5% 7%
1	G	448	3% 58% 31% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	D	844	-	-	-	X

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23793 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	418	3399	2162	580	636	3	18	0	0	0
1	B	418	3399	2162	580	636	3	18	0	0	0
1	C	418	3399	2162	580	636	3	18	0	0	0
1	D	418	3399	2162	580	636	3	18	0	0	0
1	E	418	3399	2162	580	636	3	18	0	0	0
1	F	418	3399	2162	580	636	3	18	0	0	0
1	G	418	3399	2162	580	636	3	18	0	0	0

There are 203 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	640	PRO	-	EXPRESSION TAG	UNP P32361
A	?	-	ASN	DELETION	UNP P32361
A	?	-	ASN	DELETION	UNP P32361
A	?	-	LEU	DELETION	UNP P32361
A	?	-	GLN	DELETION	UNP P32361
A	?	-	CYS	DELETION	UNP P32361
A	?	-	GLN	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	GLU	DELETION	UNP P32361
A	?	-	THR	DELETION	UNP P32361
A	?	-	GLU	DELETION	UNP P32361
A	?	-	HIS	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	DELETION	UNP P32361
A	?	-	HIS	DELETION	UNP P32361
A	?	-	THR	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	ASP	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	PHE	DELETION	UNP P32361
A	?	-	TYR	DELETION	UNP P32361
A	?	-	ASP	DELETION	UNP P32361
A	?	-	PRO	DELETION	UNP P32361
A	?	-	PHE	DELETION	UNP P32361
B	640	PRO	-	EXPRESSION TAG	UNP P32361
B	?	-	ASN	DELETION	UNP P32361
B	?	-	ASN	DELETION	UNP P32361
B	?	-	LEU	DELETION	UNP P32361
B	?	-	GLN	DELETION	UNP P32361
B	?	-	CYS	DELETION	UNP P32361
B	?	-	GLN	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	GLU	DELETION	UNP P32361
B	?	-	THR	DELETION	UNP P32361
B	?	-	GLU	DELETION	UNP P32361
B	?	-	HIS	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	ARG	DELETION	UNP P32361
B	?	-	HIS	DELETION	UNP P32361
B	?	-	THR	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	ASP	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	PHE	DELETION	UNP P32361
B	?	-	TYR	DELETION	UNP P32361
B	?	-	ASP	DELETION	UNP P32361
B	?	-	PRO	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PHE	DELETION	UNP P32361
C	640	PRO	-	EXPRESSION TAG	UNP P32361
C	?	-	ASN	DELETION	UNP P32361
C	?	-	ASN	DELETION	UNP P32361
C	?	-	LEU	DELETION	UNP P32361
C	?	-	GLN	DELETION	UNP P32361
C	?	-	CYS	DELETION	UNP P32361
C	?	-	GLN	DELETION	UNP P32361
C	?	-	VAL	DELETION	UNP P32361
C	?	-	GLU	DELETION	UNP P32361
C	?	-	THR	DELETION	UNP P32361
C	?	-	GLU	DELETION	UNP P32361
C	?	-	HIS	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	ARG	DELETION	UNP P32361
C	?	-	HIS	DELETION	UNP P32361
C	?	-	THR	DELETION	UNP P32361
C	?	-	VAL	DELETION	UNP P32361
C	?	-	VAL	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	ASP	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	PHE	DELETION	UNP P32361
C	?	-	TYR	DELETION	UNP P32361
C	?	-	ASP	DELETION	UNP P32361
C	?	-	PRO	DELETION	UNP P32361
C	?	-	PHE	DELETION	UNP P32361
D	640	PRO	-	EXPRESSION TAG	UNP P32361
D	?	-	ASN	DELETION	UNP P32361
D	?	-	ASN	DELETION	UNP P32361
D	?	-	LEU	DELETION	UNP P32361
D	?	-	GLN	DELETION	UNP P32361
D	?	-	CYS	DELETION	UNP P32361
D	?	-	GLN	DELETION	UNP P32361
D	?	-	VAL	DELETION	UNP P32361
D	?	-	GLU	DELETION	UNP P32361
D	?	-	THR	DELETION	UNP P32361
D	?	-	GLU	DELETION	UNP P32361
D	?	-	HIS	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	ARG	DELETION	UNP P32361
D	?	-	HIS	DELETION	UNP P32361
D	?	-	THR	DELETION	UNP P32361
D	?	-	VAL	DELETION	UNP P32361
D	?	-	VAL	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	ASP	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	PHE	DELETION	UNP P32361
D	?	-	TYR	DELETION	UNP P32361
D	?	-	ASP	DELETION	UNP P32361
D	?	-	PRO	DELETION	UNP P32361
D	?	-	PHE	DELETION	UNP P32361
E	640	PRO	-	EXPRESSION TAG	UNP P32361
E	?	-	ASN	DELETION	UNP P32361
E	?	-	ASN	DELETION	UNP P32361
E	?	-	LEU	DELETION	UNP P32361
E	?	-	GLN	DELETION	UNP P32361
E	?	-	CYS	DELETION	UNP P32361
E	?	-	GLN	DELETION	UNP P32361
E	?	-	VAL	DELETION	UNP P32361
E	?	-	GLU	DELETION	UNP P32361
E	?	-	THR	DELETION	UNP P32361
E	?	-	GLU	DELETION	UNP P32361
E	?	-	HIS	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	ARG	DELETION	UNP P32361
E	?	-	HIS	DELETION	UNP P32361
E	?	-	THR	DELETION	UNP P32361
E	?	-	VAL	DELETION	UNP P32361
E	?	-	VAL	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	ASP	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	PHE	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	TYR	DELETION	UNP P32361
E	?	-	ASP	DELETION	UNP P32361
E	?	-	PRO	DELETION	UNP P32361
E	?	-	PHE	DELETION	UNP P32361
F	640	PRO	-	EXPRESSION TAG	UNP P32361
F	?	-	ASN	DELETION	UNP P32361
F	?	-	ASN	DELETION	UNP P32361
F	?	-	LEU	DELETION	UNP P32361
F	?	-	GLN	DELETION	UNP P32361
F	?	-	CYS	DELETION	UNP P32361
F	?	-	GLN	DELETION	UNP P32361
F	?	-	VAL	DELETION	UNP P32361
F	?	-	GLU	DELETION	UNP P32361
F	?	-	THR	DELETION	UNP P32361
F	?	-	GLU	DELETION	UNP P32361
F	?	-	HIS	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	ARG	DELETION	UNP P32361
F	?	-	HIS	DELETION	UNP P32361
F	?	-	THR	DELETION	UNP P32361
F	?	-	VAL	DELETION	UNP P32361
F	?	-	VAL	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	ASP	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	PHE	DELETION	UNP P32361
F	?	-	TYR	DELETION	UNP P32361
F	?	-	ASP	DELETION	UNP P32361
F	?	-	PRO	DELETION	UNP P32361
F	?	-	PHE	DELETION	UNP P32361
G	640	PRO	-	EXPRESSION TAG	UNP P32361
G	?	-	ASN	DELETION	UNP P32361
G	?	-	ASN	DELETION	UNP P32361
G	?	-	LEU	DELETION	UNP P32361
G	?	-	GLN	DELETION	UNP P32361
G	?	-	CYS	DELETION	UNP P32361
G	?	-	GLN	DELETION	UNP P32361
G	?	-	VAL	DELETION	UNP P32361
G	?	-	GLU	DELETION	UNP P32361

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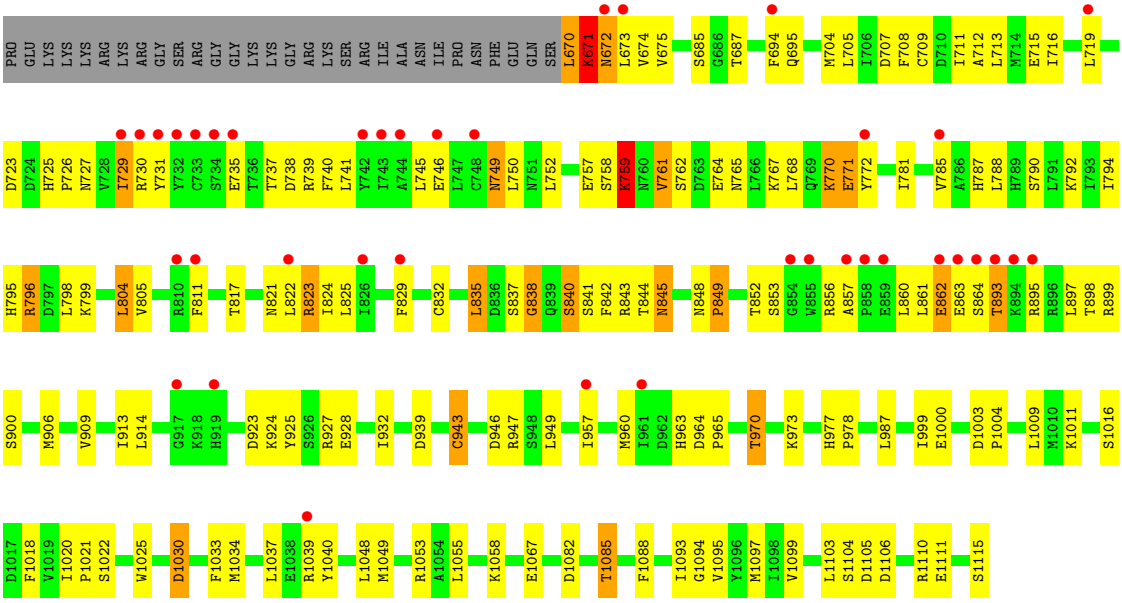
Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	THR	DELETION	UNP P32361
G	?	-	GLU	DELETION	UNP P32361
G	?	-	HIS	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	ARG	DELETION	UNP P32361
G	?	-	HIS	DELETION	UNP P32361
G	?	-	THR	DELETION	UNP P32361
G	?	-	VAL	DELETION	UNP P32361
G	?	-	VAL	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	ASP	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	PHE	DELETION	UNP P32361
G	?	-	TYR	DELETION	UNP P32361
G	?	-	ASP	DELETION	UNP P32361
G	?	-	PRO	DELETION	UNP P32361
G	?	-	PHE	DELETION	UNP P32361

3 Residue-property plots (i)

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

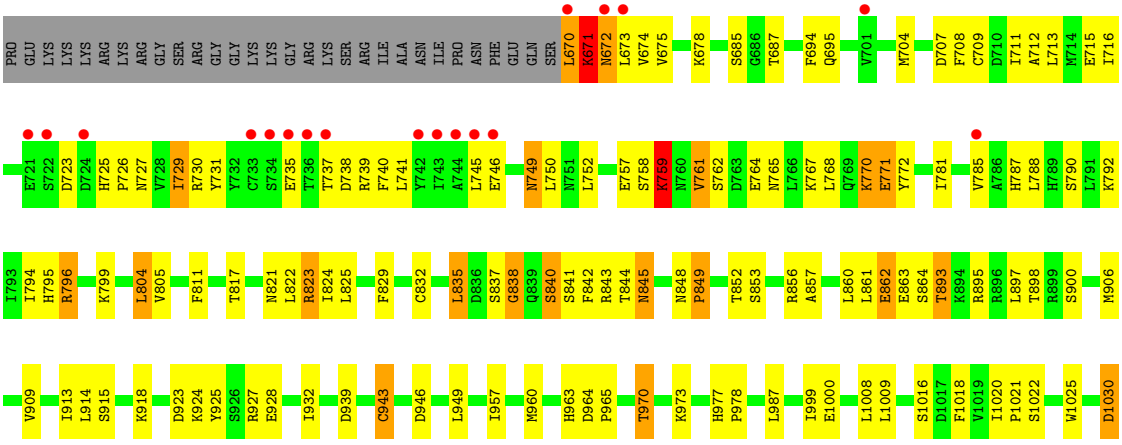
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

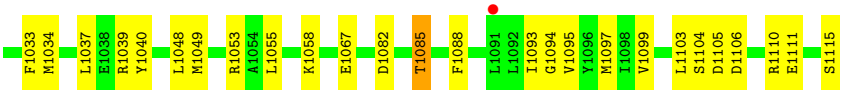
Chain A:



• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

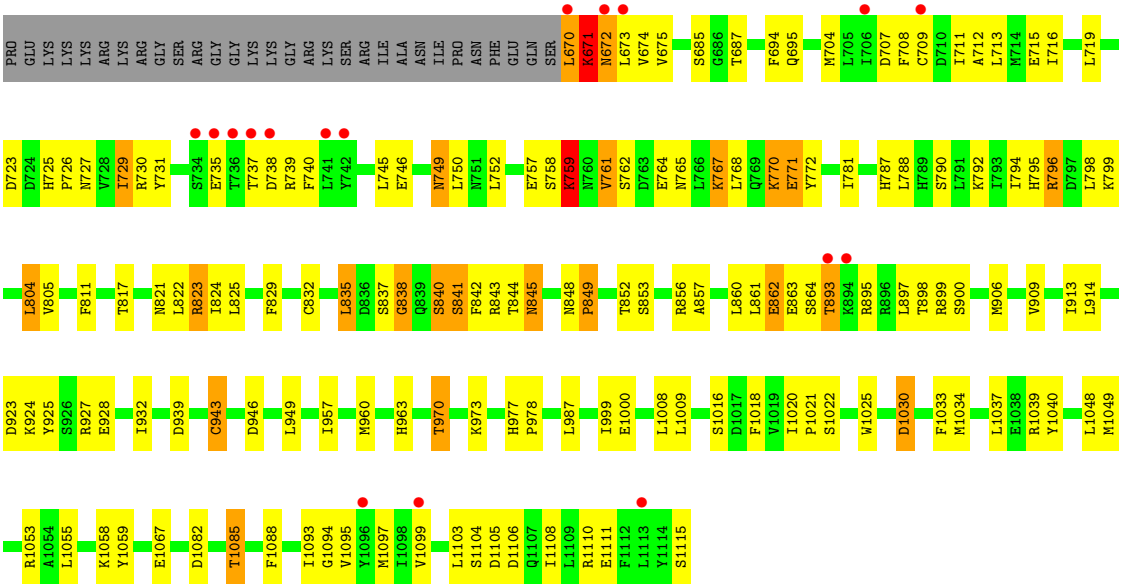
Chain B:





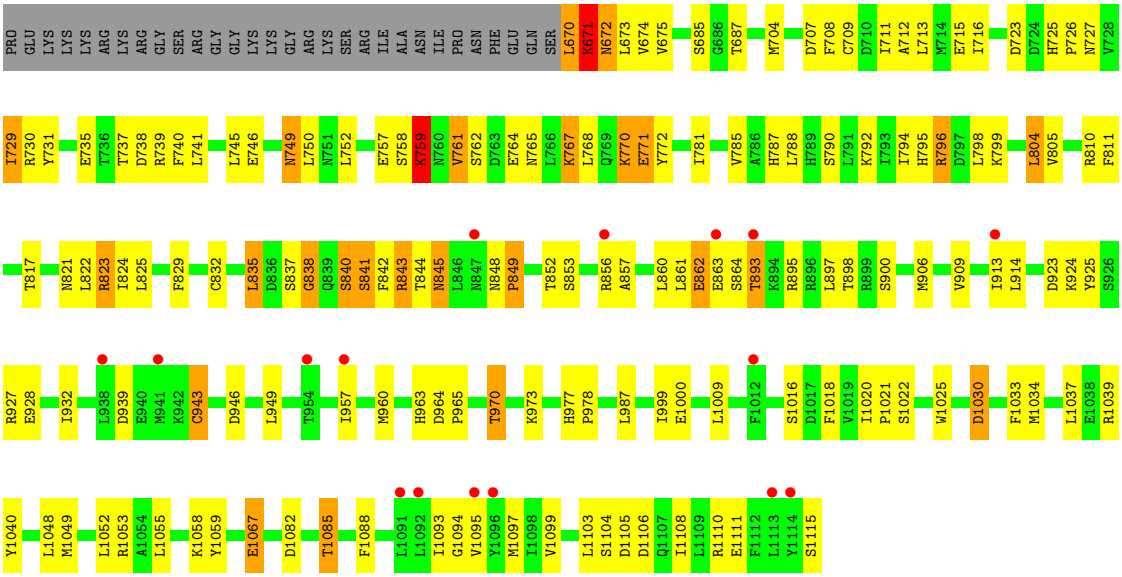
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain C:



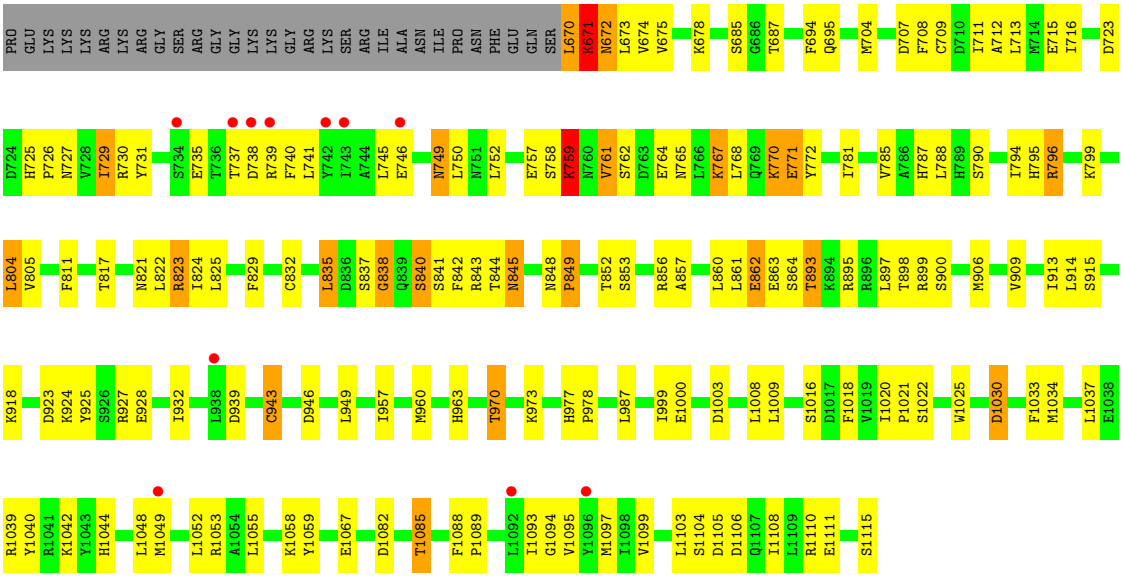
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain D:



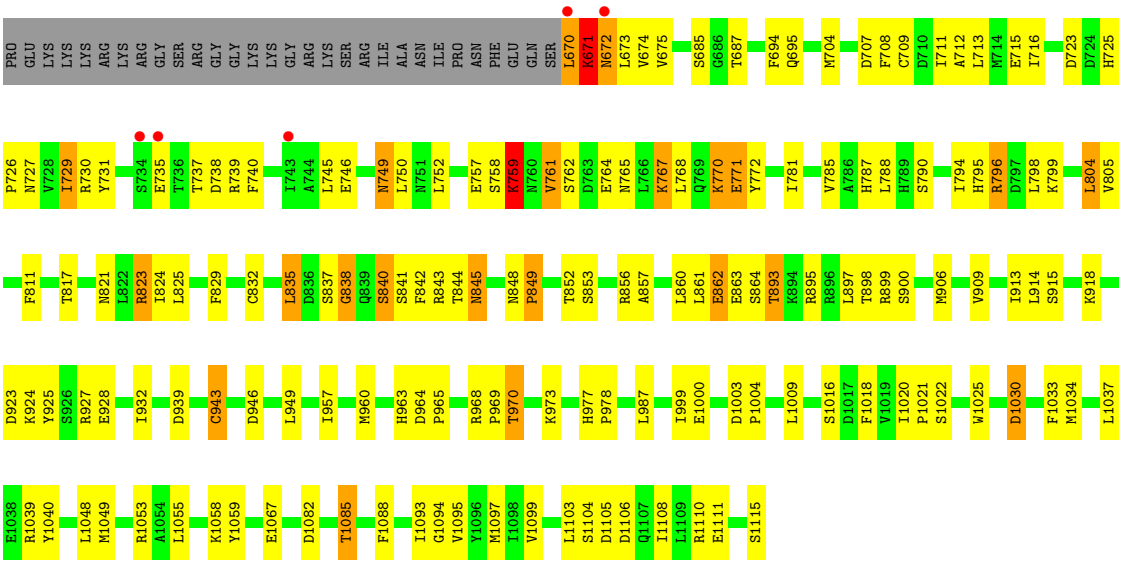
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain E:



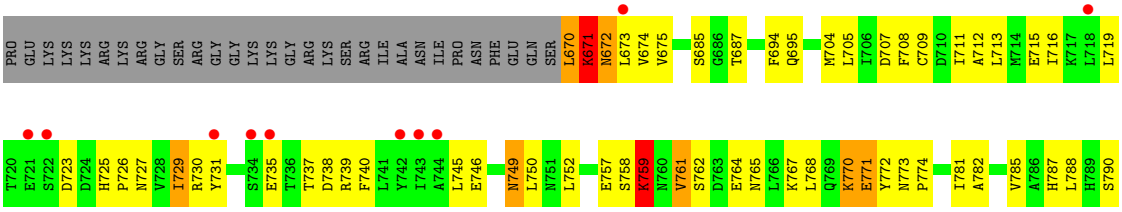
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

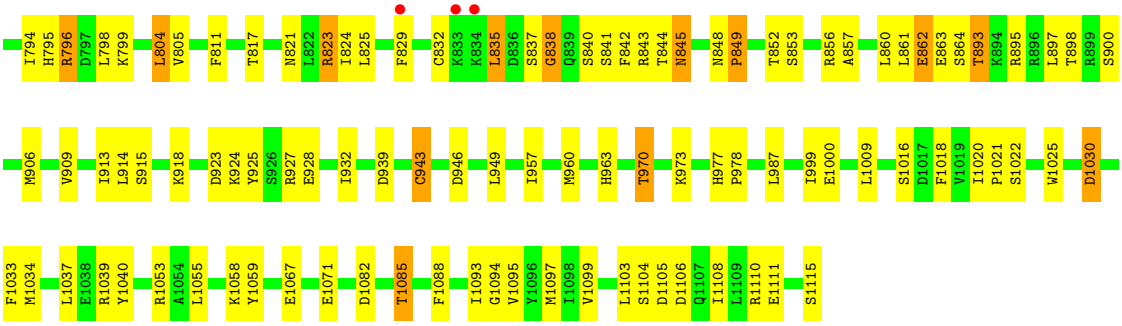
Chain F:



• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain G:




I794 H795 R796 D797 L798 K799 L804 V805 F811 T817 N821 L822 R823 I824 L825 F829 C832 K833 K834 L835 D836 S837 G838 Q839 S840 S841 F842 R843 T844 N845 N848 P849 T852 S853 R856 A857 L860 L861 E862 E863 S864 T893 K894 R895 R896 L897 T898 R899 S900
M906 V909 I913 L914 S915 K918 D923 K924 Y925 S926 R927 E928 I932 D939 C943 D946 L949 I957 M960 H963 T970 K973 H977 P978 L987 I999 E1000 L1009 S1016 D1017 F1018 V1019 I1020 P1021 S1022 W1025 D1030
F1033 M1034 L1037 E1038 R1039 Y1040 R1053 A1054 L1055 K1058 Y1059 E1067 E1071 D1082 T1085 F1088 I1093 G1094 V1095 Y1096 M1097 I1098 V1099 L1103 S1104 D1105 D1106 Q1107 I1108 L1109 R1110 E1111 S1115

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	91.65Å 580.67Å 177.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.78 – 6.60 96.78 – 6.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (96.78-6.60) 99.9 (96.78-6.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 6.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.286 , 0.317 0.283 , 0.310	Depositor DCC
R_{free} test set	471 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	344.3	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 128.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	23793	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP

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	0.35	0/3437	0.49	0/4629
1	B	0.35	0/3437	0.49	0/4629
1	C	0.35	0/3437	0.49	0/4629
1	D	0.35	0/3437	0.49	0/4629
1	E	0.35	0/3437	0.49	0/4629
1	F	0.35	0/3437	0.49	0/4629
1	G	0.35	0/3437	0.49	0/4629
All	All	0.35	0/24059	0.49	0/32403

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
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	671	LYS	Peptide
1	B	671	LYS	Peptide
1	C	671	LYS	Peptide
1	D	671	LYS	Peptide
1	E	671	LYS	Peptide
1	F	671	LYS	Peptide
1	G	671	LYS	Peptide

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	3399	0	3409	121	0
1	B	3399	0	3409	117	0
1	C	3399	0	3409	120	1
1	D	3399	0	3409	129	0
1	E	3399	0	3409	122	7
1	F	3399	0	3409	122	0
1	G	3399	0	3409	121	0
All	All	23793	0	23863	828	7

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 17.

All (828) 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:840:SEP:O2P	1:E:761:VAL:HG11	1.35	1.23
1:A:848:ASN:HB3	1:A:849:PRO:HA	1.42	1.02
1:E:848:ASN:HB3	1:E:849:PRO:HA	1.42	1.01
1:D:848:ASN:HB3	1:D:849:PRO:HA	1.42	1.01
1:B:848:ASN:HB3	1:B:849:PRO:HA	1.42	1.00
1:G:848:ASN:HB3	1:G:849:PRO:HA	1.42	0.99
1:F:848:ASN:HB3	1:F:849:PRO:HA	1.42	0.99
1:C:848:ASN:HB3	1:C:849:PRO:HA	1.42	0.98
1:D:840:SEP:O2P	1:E:761:VAL:CG1	2.23	0.86
1:C:862:GLU:HG3	1:C:863:GLU:H	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:862:GLU:HG3	1:E:863:GLU:H	1.42	0.84
1:F:862:GLU:HG3	1:F:863:GLU:H	1.42	0.84
1:A:862:GLU:HG3	1:A:863:GLU:H	1.42	0.84
1:B:862:GLU:HG3	1:B:863:GLU:H	1.42	0.83
1:D:862:GLU:HG3	1:D:863:GLU:H	1.42	0.82
1:G:862:GLU:HG3	1:G:863:GLU:H	1.42	0.82
1:B:761:VAL:HG11	1:C:840:SEP:O2P	1.86	0.76
1:F:1108:ILE:CD1	1:G:1059:TYR:OH	2.35	0.74
1:B:1034:MET:HE2	1:B:1037:LEU:HD23	1.71	0.73
1:F:715:GLU:HG3	1:F:829:PHE:HB2	1.71	0.73
1:C:715:GLU:HG3	1:C:829:PHE:HB2	1.71	0.72
1:B:715:GLU:HG3	1:B:829:PHE:HB2	1.71	0.72
1:A:1034:MET:HE1	1:A:1037:LEU:HD23	1.71	0.72
1:D:957:ILE:HA	1:D:960:MET:HE3	1.72	0.72
1:E:715:GLU:HG3	1:E:829:PHE:HB2	1.71	0.72
1:A:715:GLU:HG3	1:A:829:PHE:HB2	1.71	0.71
1:F:957:ILE:HA	1:F:960:MET:HE3	1.72	0.71
1:F:1059:TYR:OH	1:G:1108:ILE:CD1	2.38	0.71
1:G:715:GLU:HG3	1:G:829:PHE:HB2	1.71	0.71
1:C:957:ILE:HA	1:C:960:MET:HE3	1.72	0.71
1:D:715:GLU:HG3	1:D:829:PHE:HB2	1.71	0.71
1:D:1034:MET:HE2	1:D:1037:LEU:HD23	1.71	0.71
1:G:781:ILE:HG22	1:G:906:MET:HE2	1.72	0.70
1:F:1034:MET:HE2	1:F:1037:LEU:HD23	1.73	0.70
1:C:730:ARG:HB3	1:C:746:GLU:HG2	1.74	0.70
1:E:957:ILE:HA	1:E:960:MET:HE3	1.72	0.70
1:D:848:ASN:HB3	1:D:849:PRO:CA	2.21	0.70
1:E:1034:MET:HE1	1:E:1037:LEU:HD23	1.73	0.70
1:F:862:GLU:HG3	1:F:863:GLU:N	2.07	0.70
1:B:730:ARG:HB3	1:B:746:GLU:HG2	1.74	0.70
1:B:957:ILE:HA	1:B:960:MET:HE3	1.74	0.70
1:D:862:GLU:HG3	1:D:863:GLU:N	2.07	0.70
1:G:725:HIS:CD2	1:G:727:ASN:H	2.10	0.70
1:B:725:HIS:CD2	1:B:727:ASN:H	2.10	0.70
1:B:848:ASN:HB3	1:B:849:PRO:CA	2.21	0.70
1:F:730:ARG:HB3	1:F:746:GLU:HG2	1.74	0.70
1:G:862:GLU:HG3	1:G:863:GLU:N	2.07	0.70
1:A:957:ILE:HA	1:A:960:MET:HE3	1.74	0.69
1:C:725:HIS:CD2	1:C:727:ASN:H	2.10	0.69
1:C:1034:MET:HE2	1:C:1037:LEU:HD23	1.73	0.69
1:E:862:GLU:HG3	1:E:863:GLU:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:848:ASN:HB3	1:G:849:PRO:CA	2.21	0.69
1:B:862:GLU:HG3	1:B:863:GLU:N	2.07	0.69
1:G:957:ILE:HA	1:G:960:MET:HE3	1.74	0.69
1:G:1034:MET:HE2	1:G:1037:LEU:HD23	1.73	0.69
1:A:730:ARG:HB3	1:A:746:GLU:HG2	1.74	0.69
1:A:725:HIS:CD2	1:A:727:ASN:H	2.10	0.69
1:E:730:ARG:HB3	1:E:746:GLU:HG2	1.74	0.69
1:F:725:HIS:CD2	1:F:727:ASN:H	2.10	0.69
1:A:848:ASN:HB3	1:A:849:PRO:CA	2.21	0.68
1:A:862:GLU:HG3	1:A:863:GLU:N	2.07	0.68
1:C:862:GLU:HG3	1:C:863:GLU:N	2.07	0.68
1:G:730:ARG:HB3	1:G:746:GLU:HG2	1.74	0.68
1:A:795:HIS:HA	1:A:832:CYS:HB3	1.76	0.68
1:E:781:ILE:HG22	1:E:906:MET:HE2	1.76	0.68
1:E:848:ASN:HB3	1:E:849:PRO:CA	2.21	0.68
1:E:725:HIS:CD2	1:E:727:ASN:H	2.10	0.68
1:G:795:HIS:HA	1:G:832:CYS:HB3	1.76	0.68
1:D:730:ARG:HB3	1:D:746:GLU:HG2	1.74	0.68
1:D:795:HIS:HA	1:D:832:CYS:HB3	1.76	0.68
1:D:725:HIS:CD2	1:D:727:ASN:H	2.10	0.67
1:C:781:ILE:HG22	1:C:906:MET:HE2	1.75	0.67
1:F:795:HIS:HA	1:F:832:CYS:HB3	1.76	0.67
1:C:795:HIS:HA	1:C:832:CYS:HB3	1.76	0.67
1:B:795:HIS:HA	1:B:832:CYS:HB3	1.76	0.67
1:E:795:HIS:HA	1:E:832:CYS:HB3	1.76	0.66
1:F:1108:ILE:HD12	1:G:1059:TYR:OH	1.96	0.66
1:G:897:LEU:HD12	1:G:897:LEU:H	1.61	0.66
1:B:1020:ILE:HG22	1:B:1022:SER:N	2.11	0.66
1:F:1020:ILE:HG22	1:F:1022:SER:N	2.11	0.65
1:C:897:LEU:HD12	1:C:897:LEU:H	1.61	0.65
1:A:897:LEU:H	1:A:897:LEU:HD12	1.61	0.65
1:E:897:LEU:HD12	1:E:897:LEU:H	1.61	0.65
1:D:864:SER:HB3	1:D:963:HIS:NE2	2.12	0.65
1:B:897:LEU:HD12	1:B:897:LEU:H	1.61	0.65
1:D:1020:ILE:HG22	1:D:1022:SER:N	2.11	0.65
1:E:1020:ILE:HG22	1:E:1022:SER:N	2.11	0.65
1:B:781:ILE:HG22	1:B:906:MET:HE2	1.79	0.65
1:B:864:SER:HB3	1:B:963:HIS:NE2	2.12	0.65
1:F:781:ILE:HG22	1:F:906:MET:HE2	1.78	0.65
1:C:848:ASN:HB3	1:C:849:PRO:CA	2.21	0.64
1:C:864:SER:HB3	1:C:963:HIS:NE2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1020:ILE:HG22	1:G:1022:SER:N	2.11	0.64
1:A:1020:ILE:HG22	1:A:1022:SER:N	2.11	0.64
1:D:897:LEU:HD12	1:D:897:LEU:H	1.61	0.64
1:E:864:SER:HB3	1:E:963:HIS:NE2	2.12	0.64
1:C:1020:ILE:HG22	1:C:1022:SER:N	2.11	0.64
1:A:781:ILE:HG22	1:A:906:MET:HE2	1.80	0.64
1:F:864:SER:HB3	1:F:963:HIS:NE2	2.12	0.64
1:E:1034:MET:CE	1:E:1037:LEU:HD23	2.28	0.64
1:G:864:SER:HB3	1:G:963:HIS:NE2	2.12	0.64
1:D:1034:MET:CE	1:D:1037:LEU:HD23	2.28	0.64
1:B:1034:MET:CE	1:B:1037:LEU:HD23	2.28	0.63
1:A:864:SER:HB3	1:A:963:HIS:NE2	2.12	0.63
1:F:1108:ILE:HD11	1:G:1059:TYR:OH	1.96	0.63
1:G:1034:MET:CE	1:G:1037:LEU:HD23	2.28	0.63
1:C:794:ILE:HD11	1:C:835:LEU:HD12	1.81	0.63
1:F:1034:MET:CE	1:F:1037:LEU:HD23	2.28	0.63
1:G:794:ILE:HD11	1:G:835:LEU:HD12	1.81	0.63
1:A:794:ILE:HD11	1:A:835:LEU:HD12	1.81	0.62
1:C:1034:MET:CE	1:C:1037:LEU:HD23	2.28	0.62
1:D:923:ASP:O	1:D:927:ARG:HB2	1.99	0.62
1:F:897:LEU:H	1:F:897:LEU:HD12	1.61	0.62
1:B:923:ASP:O	1:B:927:ARG:HB2	1.99	0.62
1:D:794:ILE:HD11	1:D:835:LEU:HD12	1.81	0.62
1:F:923:ASP:O	1:F:927:ARG:HB2	1.99	0.62
1:A:1034:MET:CE	1:A:1037:LEU:HD23	2.28	0.62
1:B:794:ILE:HD11	1:B:835:LEU:HD12	1.81	0.62
1:G:923:ASP:O	1:G:927:ARG:HB2	1.99	0.62
1:A:923:ASP:O	1:A:927:ARG:HB2	1.99	0.62
1:C:923:ASP:O	1:C:927:ARG:HB2	1.99	0.62
1:E:923:ASP:O	1:E:927:ARG:HB2	1.99	0.62
1:C:796:ARG:HD3	1:C:832:CYS:HA	1.82	0.61
1:F:796:ARG:HD3	1:F:832:CYS:HA	1.82	0.61
1:D:781:ILE:HG22	1:D:906:MET:HE2	1.82	0.61
1:E:794:ILE:HD11	1:E:835:LEU:HD12	1.81	0.61
1:F:1059:TYR:OH	1:G:1108:ILE:HD11	1.98	0.61
1:E:796:ARG:HD3	1:E:832:CYS:HA	1.82	0.61
1:B:771:GLU:HB2	1:B:821:ASN:ND2	2.16	0.61
1:F:794:ILE:HD11	1:F:835:LEU:HD12	1.81	0.61
1:F:1059:TYR:OH	1:G:1108:ILE:HD12	1.99	0.61
1:E:771:GLU:HB2	1:E:821:ASN:ND2	2.16	0.61
1:F:771:GLU:HB2	1:F:821:ASN:ND2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:THR:HG23	1:A:973:LYS:HB2	1.83	0.61
1:C:771:GLU:HB2	1:C:821:ASN:ND2	2.16	0.61
1:B:796:ARG:HD3	1:B:832:CYS:HA	1.83	0.60
1:D:796:ARG:HD3	1:D:832:CYS:HA	1.82	0.60
1:G:796:ARG:HD3	1:G:832:CYS:HA	1.82	0.60
1:D:771:GLU:HB2	1:D:821:ASN:ND2	2.16	0.60
1:F:970:THR:HG23	1:F:973:LYS:HB2	1.83	0.60
1:A:796:ARG:HD3	1:A:832:CYS:HA	1.83	0.60
1:F:795:HIS:HA	1:F:832:CYS:CB	2.32	0.60
1:G:970:THR:HG23	1:G:973:LYS:HB2	1.83	0.60
1:A:771:GLU:HB2	1:A:821:ASN:ND2	2.16	0.60
1:C:970:THR:HG23	1:C:973:LYS:HB2	1.83	0.60
1:E:795:HIS:HA	1:E:832:CYS:CB	2.32	0.60
1:G:771:GLU:HB2	1:G:821:ASN:ND2	2.16	0.60
1:B:970:THR:HG23	1:B:973:LYS:HB2	1.83	0.59
1:B:795:HIS:HA	1:B:832:CYS:CB	2.32	0.59
1:C:795:HIS:HA	1:C:832:CYS:CB	2.32	0.59
1:D:840:SEP:P	1:E:761:VAL:HG11	2.41	0.59
1:E:970:THR:HG23	1:E:973:LYS:HB2	1.83	0.59
1:D:761:VAL:HG21	1:D:764:GLU:HG3	1.85	0.59
1:D:970:THR:HG23	1:D:973:LYS:HB2	1.83	0.59
1:D:795:HIS:HA	1:D:832:CYS:CB	2.32	0.59
1:G:795:HIS:HA	1:G:832:CYS:CB	2.32	0.59
1:C:772:TYR:CG	1:C:772:TYR:O	2.56	0.59
1:F:761:VAL:HG21	1:F:764:GLU:HG3	1.85	0.59
1:B:772:TYR:CG	1:B:772:TYR:O	2.56	0.59
1:C:761:VAL:HG21	1:C:764:GLU:HG3	1.85	0.59
1:D:771:GLU:HB2	1:D:821:ASN:HD21	1.68	0.58
1:E:772:TYR:CG	1:E:772:TYR:O	2.56	0.58
1:G:771:GLU:HB2	1:G:821:ASN:HD21	1.68	0.58
1:A:772:TYR:O	1:A:772:TYR:CG	2.56	0.58
1:A:795:HIS:HA	1:A:832:CYS:CB	2.32	0.58
1:A:771:GLU:HB2	1:A:821:ASN:HD21	1.68	0.58
1:B:771:GLU:HB2	1:B:821:ASN:HD21	1.68	0.58
1:C:771:GLU:HB2	1:C:821:ASN:HD21	1.68	0.58
1:D:772:TYR:CG	1:D:772:TYR:O	2.56	0.58
1:F:771:GLU:HB2	1:F:821:ASN:HD21	1.68	0.58
1:G:861:LEU:O	1:G:862:GLU:HB3	2.04	0.58
1:E:761:VAL:HG21	1:E:764:GLU:HG3	1.85	0.58
1:F:772:TYR:O	1:F:772:TYR:CG	2.56	0.58
1:F:848:ASN:HB3	1:F:849:PRO:CA	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:VAL:HG21	1:A:764:GLU:HG3	1.85	0.58
1:A:861:LEU:O	1:A:862:GLU:HB3	2.04	0.57
1:B:861:LEU:O	1:B:862:GLU:HB3	2.04	0.57
1:C:861:LEU:O	1:C:862:GLU:HB3	2.04	0.57
1:B:761:VAL:HG21	1:B:764:GLU:HG3	1.85	0.57
1:F:861:LEU:O	1:F:862:GLU:HB3	2.04	0.57
1:E:771:GLU:HB2	1:E:821:ASN:HD21	1.68	0.57
1:E:861:LEU:O	1:E:862:GLU:HB3	2.04	0.57
1:G:772:TYR:CG	1:G:772:TYR:O	2.56	0.57
1:D:861:LEU:O	1:D:862:GLU:HB3	2.04	0.57
1:G:781:ILE:HG12	1:G:824:ILE:HG21	1.87	0.57
1:A:781:ILE:HG12	1:A:824:ILE:HG21	1.87	0.56
1:B:781:ILE:HG12	1:B:824:ILE:HG21	1.87	0.56
1:D:781:ILE:HG12	1:D:824:ILE:HG21	1.87	0.56
1:A:897:LEU:HD12	1:A:897:LEU:N	2.20	0.56
1:D:897:LEU:HD12	1:D:897:LEU:N	2.20	0.56
1:G:761:VAL:HG21	1:G:764:GLU:HG3	1.85	0.56
1:B:709:CYS:O	1:B:713:LEU:HD13	2.06	0.56
1:E:709:CYS:O	1:E:713:LEU:HD13	2.06	0.56
1:C:781:ILE:HG12	1:C:824:ILE:HG21	1.87	0.56
1:A:709:CYS:O	1:A:713:LEU:HD13	2.06	0.56
1:G:897:LEU:HD12	1:G:897:LEU:N	2.20	0.56
1:E:749:ASN:OD1	1:E:749:ASN:N	2.39	0.56
1:E:897:LEU:HD12	1:E:897:LEU:N	2.20	0.56
1:B:897:LEU:HD12	1:B:897:LEU:N	2.20	0.56
1:F:709:CYS:O	1:F:713:LEU:HD13	2.06	0.56
1:G:709:CYS:O	1:G:713:LEU:HD13	2.06	0.56
1:E:781:ILE:HG12	1:E:824:ILE:HG21	1.87	0.56
1:D:709:CYS:O	1:D:713:LEU:HD13	2.06	0.55
1:A:749:ASN:OD1	1:A:749:ASN:N	2.39	0.55
1:F:897:LEU:HD12	1:F:897:LEU:N	2.20	0.55
1:F:781:ILE:HG12	1:F:824:ILE:HG21	1.87	0.55
1:C:897:LEU:HD12	1:C:897:LEU:N	2.20	0.55
1:C:709:CYS:O	1:C:713:LEU:HD13	2.06	0.55
1:B:757:GLU:O	1:B:759:LYS:HE3	2.07	0.55
1:C:749:ASN:OD1	1:C:749:ASN:N	2.39	0.55
1:E:757:GLU:O	1:E:759:LYS:HE3	2.07	0.54
1:G:757:GLU:O	1:G:759:LYS:HE3	2.07	0.54
1:F:749:ASN:OD1	1:F:749:ASN:N	2.39	0.54
1:F:752:LEU:HD21	1:F:913:ILE:HD11	1.90	0.54
1:B:752:LEU:HD21	1:B:913:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:LEU:HD21	1:A:913:ILE:HD11	1.90	0.54
1:C:737:THR:HG23	1:C:740:PHE:H	1.73	0.54
1:E:824:ILE:O	1:E:825:LEU:HD23	2.08	0.54
1:A:757:GLU:O	1:A:759:LYS:HE3	2.07	0.54
1:D:824:ILE:O	1:D:825:LEU:HD23	2.08	0.54
1:A:737:THR:HG23	1:A:740:PHE:H	1.73	0.54
1:C:752:LEU:HD21	1:C:913:ILE:HD11	1.90	0.54
1:E:737:THR:HG23	1:E:740:PHE:H	1.73	0.54
1:E:752:LEU:HD21	1:E:913:ILE:HD11	1.90	0.54
1:G:737:THR:HG23	1:G:740:PHE:H	1.73	0.54
1:G:749:ASN:OD1	1:G:749:ASN:N	2.39	0.54
1:G:1055:LEU:HD23	1:G:1055:LEU:C	2.29	0.54
1:A:824:ILE:O	1:A:825:LEU:HD23	2.08	0.54
1:B:1055:LEU:C	1:B:1055:LEU:HD23	2.29	0.54
1:D:671:LYS:HD2	1:D:671:LYS:O	2.08	0.54
1:D:1055:LEU:C	1:D:1055:LEU:HD23	2.29	0.54
1:E:1055:LEU:HD23	1:E:1055:LEU:C	2.29	0.54
1:C:757:GLU:O	1:C:759:LYS:HE3	2.07	0.54
1:D:757:GLU:O	1:D:759:LYS:HE3	2.07	0.54
1:D:749:ASN:OD1	1:D:749:ASN:N	2.39	0.53
1:E:909:VAL:O	1:E:913:ILE:HG12	2.08	0.53
1:F:909:VAL:O	1:F:913:ILE:HG12	2.09	0.53
1:C:671:LYS:HD2	1:C:671:LYS:O	2.08	0.53
1:C:824:ILE:O	1:C:825:LEU:HD23	2.08	0.53
1:C:909:VAL:O	1:C:913:ILE:HG12	2.08	0.53
1:D:909:VAL:O	1:D:913:ILE:HG12	2.08	0.53
1:D:1111:GLU:O	1:D:1115:SER:HB3	2.09	0.53
1:F:757:GLU:O	1:F:759:LYS:HE3	2.07	0.53
1:F:824:ILE:O	1:F:825:LEU:HD23	2.08	0.53
1:F:1111:GLU:O	1:F:1115:SER:HB3	2.09	0.53
1:G:1111:GLU:O	1:G:1115:SER:HB3	2.09	0.53
1:A:723:ASP:HB2	1:A:730:ARG:HA	1.91	0.53
1:B:737:THR:HG23	1:B:740:PHE:H	1.73	0.53
1:B:1111:GLU:O	1:B:1115:SER:HB3	2.09	0.53
1:C:1111:GLU:O	1:C:1115:SER:HB3	2.09	0.53
1:E:1111:GLU:O	1:E:1115:SER:HB3	2.09	0.53
1:G:723:ASP:HB2	1:G:730:ARG:HA	1.91	0.53
1:B:909:VAL:O	1:B:913:ILE:HG12	2.08	0.53
1:B:1093:ILE:O	1:B:1097:MET:HG3	2.09	0.53
1:C:1055:LEU:C	1:C:1055:LEU:HD23	2.29	0.53
1:E:723:ASP:HB2	1:E:730:ARG:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:671:LYS:HD2	1:F:671:LYS:O	2.08	0.53
1:F:737:THR:HG23	1:F:740:PHE:H	1.73	0.53
1:G:671:LYS:HD2	1:G:671:LYS:O	2.08	0.53
1:A:1055:LEU:C	1:A:1055:LEU:HD23	2.29	0.53
1:B:671:LYS:HD2	1:B:671:LYS:O	2.08	0.53
1:G:752:LEU:HD21	1:G:913:ILE:HD11	1.90	0.53
1:A:671:LYS:HD2	1:A:671:LYS:O	2.08	0.53
1:G:824:ILE:O	1:G:825:LEU:HD23	2.08	0.53
1:A:909:VAL:O	1:A:913:ILE:HG12	2.09	0.53
1:A:1093:ILE:O	1:A:1097:MET:HG3	2.09	0.53
1:B:824:ILE:O	1:B:825:LEU:HD23	2.08	0.53
1:D:752:LEU:HD21	1:D:913:ILE:HD11	1.90	0.53
1:F:1055:LEU:C	1:F:1055:LEU:HD23	2.29	0.53
1:A:1111:GLU:O	1:A:1115:SER:HB3	2.09	0.52
1:C:1093:ILE:O	1:C:1097:MET:HG3	2.09	0.52
1:F:1093:ILE:O	1:F:1097:MET:HG3	2.09	0.52
1:B:723:ASP:HB2	1:B:730:ARG:HA	1.91	0.52
1:A:928:GLU:O	1:A:932:ILE:HG13	2.10	0.52
1:E:671:LYS:HD2	1:E:671:LYS:O	2.08	0.52
1:E:1093:ILE:O	1:E:1097:MET:HG3	2.09	0.52
1:G:909:VAL:O	1:G:913:ILE:HG12	2.09	0.52
1:D:928:GLU:O	1:D:932:ILE:HG13	2.10	0.52
1:D:1034:MET:HE3	1:D:1034:MET:HA	1.91	0.52
1:F:928:GLU:O	1:F:932:ILE:HG13	2.10	0.52
1:G:928:GLU:O	1:G:932:ILE:HG13	2.10	0.52
1:D:731:TYR:HA	1:D:745:LEU:HD23	1.92	0.52
1:D:1093:ILE:O	1:D:1097:MET:HG3	2.09	0.52
1:A:1034:MET:HE2	1:A:1034:MET:HA	1.92	0.52
1:B:749:ASN:OD1	1:B:749:ASN:N	2.39	0.52
1:B:1034:MET:HA	1:B:1034:MET:HE3	1.91	0.52
1:C:928:GLU:O	1:C:932:ILE:HG13	2.10	0.52
1:D:723:ASP:HB2	1:D:730:ARG:HA	1.91	0.52
1:D:729:ILE:CD1	1:D:745:LEU:HB3	2.40	0.52
1:B:729:ILE:CD1	1:B:745:LEU:HB3	2.40	0.52
1:C:731:TYR:HA	1:C:745:LEU:HD23	1.92	0.52
1:D:737:THR:HG23	1:D:740:PHE:H	1.73	0.52
1:G:729:ILE:CD1	1:G:745:LEU:HB3	2.40	0.52
1:G:1093:ILE:O	1:G:1097:MET:HG3	2.09	0.52
1:A:729:ILE:CD1	1:A:745:LEU:HB3	2.40	0.51
1:C:729:ILE:CD1	1:C:745:LEU:HB3	2.40	0.51
1:F:723:ASP:HB2	1:F:730:ARG:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:729:ILE:CD1	1:F:745:LEU:HB3	2.40	0.51
1:F:731:TYR:HA	1:F:745:LEU:HD23	1.92	0.51
1:A:840:SEP:O2P	1:D:761:VAL:HG11	2.10	0.51
1:E:729:ILE:CD1	1:E:745:LEU:HB3	2.40	0.51
1:A:731:TYR:HA	1:A:745:LEU:HD23	1.92	0.51
1:B:731:TYR:HA	1:B:745:LEU:HD23	1.92	0.51
1:C:723:ASP:HB2	1:C:730:ARG:HA	1.91	0.51
1:B:928:GLU:O	1:B:932:ILE:HG13	2.10	0.51
1:B:811:PHE:HB3	1:B:823:ARG:NH1	2.26	0.51
1:B:861:LEU:O	1:B:862:GLU:CB	2.59	0.51
1:E:731:TYR:HA	1:E:745:LEU:HD23	1.92	0.51
1:F:811:PHE:HB3	1:F:823:ARG:NH1	2.26	0.51
1:G:845:ASN:HD22	1:G:845:ASN:N	2.08	0.51
1:E:811:PHE:HB3	1:E:823:ARG:NH1	2.26	0.51
1:C:758:SER:HB3	1:C:768:LEU:HD21	1.93	0.51
1:C:853:SER:HA	1:C:856:ARG:HG3	1.93	0.51
1:A:1000:GLU:HB2	1:A:1009:LEU:HD21	1.93	0.51
1:B:758:SER:HB3	1:B:768:LEU:HD21	1.93	0.51
1:C:781:ILE:HG22	1:C:906:MET:CE	2.41	0.51
1:C:1059:TYR:OH	1:D:1108:ILE:CD1	2.58	0.51
1:D:811:PHE:HB3	1:D:823:ARG:NH1	2.26	0.51
1:E:928:GLU:O	1:E:932:ILE:HG13	2.10	0.51
1:F:1000:GLU:HB2	1:F:1009:LEU:HD21	1.93	0.51
1:A:811:PHE:HB3	1:A:823:ARG:NH1	2.26	0.50
1:C:837:SER:HB3	1:C:838:GLY:HA2	1.93	0.50
1:D:861:LEU:O	1:D:862:GLU:CB	2.59	0.50
1:E:758:SER:HB3	1:E:768:LEU:HD21	1.93	0.50
1:F:837:SER:HB3	1:F:838:GLY:HA2	1.93	0.50
1:G:853:SER:HA	1:G:856:ARG:HG3	1.93	0.50
1:A:794:ILE:HG22	1:A:795:HIS:O	2.12	0.50
1:C:811:PHE:HB3	1:C:823:ARG:NH1	2.26	0.50
1:E:1000:GLU:HB2	1:E:1009:LEU:HD21	1.93	0.50
1:G:811:PHE:HB3	1:G:823:ARG:NH1	2.26	0.50
1:A:837:SER:HB3	1:A:838:GLY:HA2	1.94	0.50
1:F:758:SER:HB3	1:F:768:LEU:HD21	1.93	0.50
1:B:1034:MET:CE	1:B:1034:MET:HA	2.42	0.50
1:F:845:ASN:N	1:F:845:ASN:HD22	2.08	0.50
1:G:794:ILE:HG22	1:G:795:HIS:O	2.12	0.50
1:B:1000:GLU:HB2	1:B:1009:LEU:HD21	1.93	0.50
1:C:861:LEU:O	1:C:862:GLU:CB	2.59	0.50
1:E:781:ILE:HG22	1:E:906:MET:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:864:SER:O	1:E:893:THR:OG1	2.29	0.50
1:E:1034:MET:CE	1:E:1034:MET:HA	2.42	0.50
1:F:848:ASN:CB	1:F:849:PRO:HA	2.29	0.50
1:G:1000:GLU:HB2	1:G:1009:LEU:HD21	1.93	0.50
1:A:845:ASN:N	1:A:845:ASN:HD22	2.08	0.50
1:C:794:ILE:HG22	1:C:795:HIS:O	2.12	0.50
1:D:758:SER:HB3	1:D:768:LEU:HD21	1.93	0.50
1:E:794:ILE:HG22	1:E:795:HIS:O	2.12	0.50
1:F:781:ILE:HG22	1:F:906:MET:CE	2.41	0.50
1:G:758:SER:HB3	1:G:768:LEU:HD21	1.93	0.50
1:A:1034:MET:CE	1:A:1034:MET:HA	2.42	0.50
1:B:1016:SER:C	1:B:1018:PHE:H	2.15	0.50
1:E:845:ASN:N	1:E:845:ASN:HD22	2.08	0.50
1:G:1016:SER:C	1:G:1018:PHE:H	2.15	0.50
1:C:845:ASN:N	1:C:845:ASN:HD22	2.08	0.50
1:A:861:LEU:O	1:A:862:GLU:CB	2.59	0.49
1:B:781:ILE:HG22	1:B:906:MET:CE	2.41	0.49
1:B:794:ILE:HG22	1:B:795:HIS:O	2.12	0.49
1:B:845:ASN:N	1:B:845:ASN:HD22	2.08	0.49
1:B:853:SER:HA	1:B:856:ARG:HG3	1.93	0.49
1:D:924:LYS:HG3	1:D:925:TYR:CD2	2.47	0.49
1:E:861:LEU:O	1:E:862:GLU:CB	2.59	0.49
1:G:837:SER:HB3	1:G:838:GLY:HA2	1.94	0.49
1:G:1034:MET:CE	1:G:1034:MET:HA	2.42	0.49
1:G:781:ILE:HG22	1:G:906:MET:CE	2.41	0.49
1:A:924:LYS:HG3	1:A:925:TYR:CD2	2.47	0.49
1:D:853:SER:HA	1:D:856:ARG:HG3	1.93	0.49
1:E:853:SER:HA	1:E:856:ARG:HG3	1.93	0.49
1:F:1034:MET:CE	1:F:1034:MET:HA	2.42	0.49
1:G:731:TYR:HA	1:G:745:LEU:HD23	1.92	0.49
1:A:781:ILE:HG22	1:A:906:MET:CE	2.41	0.49
1:A:1016:SER:C	1:A:1018:PHE:H	2.15	0.49
1:C:1016:SER:C	1:C:1018:PHE:H	2.15	0.49
1:D:845:ASN:N	1:D:845:ASN:HD22	2.08	0.49
1:E:673:LEU:HD23	1:E:673:LEU:C	2.33	0.49
1:F:673:LEU:C	1:F:673:LEU:HD23	2.33	0.49
1:F:853:SER:HA	1:F:856:ARG:HG3	1.93	0.49
1:G:861:LEU:O	1:G:862:GLU:CB	2.59	0.49
1:G:924:LYS:HG3	1:G:925:TYR:CD2	2.48	0.49
1:A:758:SER:HB3	1:A:768:LEU:HD21	1.93	0.49
1:A:864:SER:O	1:A:893:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:837:SER:HB3	1:B:838:GLY:HA2	1.94	0.49
1:C:924:LYS:HG3	1:C:925:TYR:CD2	2.47	0.49
1:C:1108:ILE:CD1	1:D:1059:TYR:OH	2.59	0.49
1:D:781:ILE:HG22	1:D:906:MET:CE	2.41	0.49
1:D:837:SER:HB3	1:D:838:GLY:HA2	1.94	0.49
1:D:1000:GLU:HB2	1:D:1009:LEU:HD21	1.93	0.49
1:F:924:LYS:HG3	1:F:925:TYR:CD2	2.47	0.49
1:D:673:LEU:C	1:D:673:LEU:HD23	2.33	0.49
1:F:861:LEU:O	1:F:862:GLU:CB	2.59	0.49
1:A:853:SER:HA	1:A:856:ARG:HG3	1.93	0.49
1:D:794:ILE:HG22	1:D:795:HIS:O	2.12	0.49
1:G:673:LEU:HD23	1:G:673:LEU:C	2.33	0.49
1:D:1034:MET:CE	1:D:1034:MET:HA	2.42	0.49
1:E:924:LYS:HG3	1:E:925:TYR:CD2	2.47	0.49
1:A:947:ARG:HB2	1:G:1071:GLU:OE1	2.13	0.49
1:B:673:LEU:HD23	1:B:673:LEU:C	2.33	0.49
1:C:1000:GLU:HB2	1:C:1009:LEU:HD21	1.93	0.49
1:C:1034:MET:CE	1:C:1034:MET:HA	2.42	0.49
1:D:1016:SER:C	1:D:1018:PHE:H	2.15	0.49
1:B:924:LYS:HG3	1:B:925:TYR:CD2	2.47	0.48
1:C:673:LEU:C	1:C:673:LEU:HD23	2.33	0.48
1:C:770:LYS:HG2	1:C:771:GLU:N	2.28	0.48
1:E:837:SER:HB3	1:E:838:GLY:HA2	1.93	0.48
1:E:1016:SER:C	1:E:1018:PHE:H	2.15	0.48
1:G:970:THR:HG23	1:G:973:LYS:CB	2.43	0.48
1:C:864:SER:O	1:C:893:THR:OG1	2.29	0.48
1:D:674:VAL:CG1	1:D:675:VAL:N	2.76	0.48
1:F:794:ILE:HG22	1:F:795:HIS:O	2.12	0.48
1:D:770:LYS:HG2	1:D:771:GLU:N	2.28	0.48
1:E:770:LYS:HG2	1:E:771:GLU:N	2.28	0.48
1:A:673:LEU:C	1:A:673:LEU:HD23	2.33	0.48
1:D:970:THR:HG23	1:D:973:LYS:CB	2.44	0.48
1:F:1016:SER:C	1:F:1018:PHE:H	2.15	0.48
1:A:674:VAL:CG1	1:A:675:VAL:N	2.76	0.48
1:A:893:THR:O	1:A:895:ARG:HG3	2.14	0.48
1:B:1025:TRP:HB2	1:B:1088:PHE:CZ	2.49	0.48
1:F:893:THR:O	1:F:895:ARG:HG3	2.14	0.48
1:B:970:THR:HG23	1:B:973:LYS:CB	2.43	0.48
1:B:770:LYS:HG2	1:B:771:GLU:N	2.28	0.48
1:C:893:THR:O	1:C:895:ARG:HG3	2.14	0.48
1:G:893:THR:O	1:G:895:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:LYS:HG2	1:A:771:GLU:N	2.28	0.48
1:A:1025:TRP:HB2	1:A:1088:PHE:CZ	2.49	0.48
1:C:1025:TRP:HB2	1:C:1088:PHE:CZ	2.49	0.48
1:D:864:SER:O	1:D:893:THR:OG1	2.29	0.48
1:C:977:HIS:CG	1:C:978:PRO:HD2	2.49	0.48
1:E:893:THR:O	1:E:895:ARG:HG3	2.14	0.48
1:E:977:HIS:CG	1:E:978:PRO:HD2	2.49	0.48
1:F:770:LYS:HG2	1:F:771:GLU:N	2.28	0.48
1:G:864:SER:O	1:G:893:THR:OG1	2.29	0.48
1:A:977:HIS:CG	1:A:978:PRO:HD2	2.49	0.47
1:D:893:THR:O	1:D:895:ARG:HG3	2.14	0.47
1:G:674:VAL:CG1	1:G:675:VAL:N	2.76	0.47
1:A:719:LEU:HD23	1:A:719:LEU:HA	1.71	0.47
1:A:970:THR:HG23	1:A:973:LYS:CB	2.44	0.47
1:B:893:THR:O	1:B:895:ARG:HG3	2.14	0.47
1:E:970:THR:HG23	1:E:973:LYS:CB	2.43	0.47
1:C:674:VAL:CG1	1:C:675:VAL:N	2.76	0.47
1:E:674:VAL:CG1	1:E:675:VAL:N	2.76	0.47
1:G:770:LYS:HG2	1:G:771:GLU:N	2.28	0.47
1:C:1034:MET:HA	1:C:1034:MET:HE3	1.96	0.47
1:D:841:SEP:O2P	1:E:678:LYS:HE3	2.13	0.47
1:D:1025:TRP:HB2	1:D:1088:PHE:CZ	2.49	0.47
1:F:674:VAL:CG1	1:F:675:VAL:N	2.76	0.47
1:F:970:THR:HG23	1:F:973:LYS:CB	2.44	0.47
1:C:1059:TYR:OH	1:D:1108:ILE:HD12	2.14	0.47
1:E:1025:TRP:HB2	1:E:1088:PHE:CZ	2.49	0.47
1:B:674:VAL:CG1	1:B:675:VAL:N	2.76	0.47
1:B:804:LEU:HB2	1:B:825:LEU:HB2	1.97	0.47
1:D:725:HIS:CG	1:D:726:PRO:HD2	2.50	0.47
1:D:804:LEU:HB2	1:D:825:LEU:HB2	1.97	0.47
1:F:977:HIS:CG	1:F:978:PRO:HD2	2.49	0.47
1:F:1025:TRP:HB2	1:F:1088:PHE:CZ	2.49	0.47
1:G:1025:TRP:HB2	1:G:1088:PHE:CZ	2.49	0.47
1:A:672:ASN:H	1:A:672:ASN:ND2	2.13	0.47
1:C:672:ASN:ND2	1:C:672:ASN:H	2.13	0.47
1:D:977:HIS:CG	1:D:978:PRO:HD2	2.49	0.47
1:F:672:ASN:H	1:F:672:ASN:ND2	2.13	0.47
1:G:977:HIS:CG	1:G:978:PRO:HD2	2.49	0.47
1:B:725:HIS:CG	1:B:726:PRO:HD2	2.50	0.47
1:C:837:SER:CB	1:C:838:GLY:HA2	2.45	0.47
1:F:804:LEU:HB2	1:F:825:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:837:SER:CB	1:F:838:GLY:HA2	2.45	0.47
1:B:672:ASN:H	1:B:672:ASN:ND2	2.13	0.47
1:B:977:HIS:CG	1:B:978:PRO:HD2	2.49	0.47
1:B:1037:LEU:C	1:B:1039:ARG:H	2.18	0.47
1:C:1037:LEU:C	1:C:1039:ARG:H	2.18	0.47
1:D:837:SER:CB	1:D:838:GLY:HA2	2.45	0.47
1:F:842:PHE:O	1:F:842:PHE:CG	2.68	0.47
1:F:1034:MET:HA	1:F:1034:MET:HE3	1.97	0.47
1:A:1037:LEU:C	1:A:1039:ARG:H	2.18	0.46
1:C:970:THR:HG23	1:C:973:LYS:CB	2.44	0.46
1:E:1034:MET:HA	1:E:1034:MET:HE2	1.97	0.46
1:A:725:HIS:CG	1:A:726:PRO:HD2	2.50	0.46
1:A:737:THR:C	1:A:739:ARG:H	2.19	0.46
1:A:837:SER:CB	1:A:838:GLY:HA2	2.45	0.46
1:B:737:THR:C	1:B:739:ARG:H	2.19	0.46
1:C:804:LEU:HB2	1:C:825:LEU:HB2	1.97	0.46
1:D:906:MET:HE3	1:D:906:MET:HB2	1.76	0.46
1:F:737:THR:C	1:F:739:ARG:H	2.19	0.46
1:A:804:LEU:HB2	1:A:825:LEU:HB2	1.97	0.46
1:B:687:THR:HG23	1:B:704:MET:HG2	1.98	0.46
1:D:1037:LEU:C	1:D:1039:ARG:H	2.18	0.46
1:E:906:MET:HE3	1:E:906:MET:HB2	1.77	0.46
1:F:725:HIS:CG	1:F:726:PRO:HD2	2.50	0.46
1:G:725:HIS:CG	1:G:726:PRO:HD2	2.50	0.46
1:A:914:LEU:O	1:A:943:CYS:HB2	2.16	0.46
1:E:725:HIS:CG	1:E:726:PRO:HD2	2.50	0.46
1:G:737:THR:C	1:G:739:ARG:H	2.19	0.46
1:G:1034:MET:HA	1:G:1034:MET:HE3	1.97	0.46
1:A:740:PHE:HB3	1:A:741:LEU:H	1.63	0.46
1:C:842:PHE:CG	1:C:842:PHE:O	2.68	0.46
1:D:672:ASN:H	1:D:672:ASN:ND2	2.13	0.46
1:D:737:THR:C	1:D:739:ARG:H	2.19	0.46
1:D:857:ALA:O	1:D:860:LEU:HB2	2.16	0.46
1:E:837:SER:CB	1:E:838:GLY:HA2	2.45	0.46
1:A:794:ILE:O	1:A:832:CYS:HB2	2.16	0.46
1:B:837:SER:CB	1:B:838:GLY:HA2	2.45	0.46
1:C:1108:ILE:HD12	1:D:1059:TYR:OH	2.15	0.46
1:D:687:THR:HG23	1:D:704:MET:HG2	1.98	0.46
1:B:864:SER:O	1:B:893:THR:OG1	2.29	0.46
1:D:794:ILE:O	1:D:832:CYS:HB2	2.16	0.46
1:G:794:ILE:O	1:G:832:CYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:837:SER:CB	1:G:838:GLY:HA2	2.45	0.46
1:G:1037:LEU:C	1:G:1039:ARG:H	2.18	0.46
1:B:794:ILE:O	1:B:832:CYS:HB2	2.16	0.46
1:B:842:PHE:CG	1:B:842:PHE:O	2.68	0.46
1:B:914:LEU:O	1:B:943:CYS:HB2	2.16	0.46
1:C:914:LEU:O	1:C:943:CYS:HB2	2.16	0.46
1:E:687:THR:HG23	1:E:704:MET:HG2	1.98	0.46
1:G:914:LEU:O	1:G:943:CYS:HB2	2.16	0.46
1:B:857:ALA:O	1:B:860:LEU:HB2	2.16	0.46
1:C:737:THR:C	1:C:739:ARG:H	2.19	0.46
1:D:785:VAL:HG21	1:D:906:MET:HE1	1.97	0.46
1:D:914:LEU:O	1:D:943:CYS:HB2	2.16	0.46
1:E:804:LEU:HB2	1:E:825:LEU:HB2	1.97	0.46
1:E:842:PHE:CG	1:E:842:PHE:O	2.68	0.46
1:G:804:LEU:HB2	1:G:825:LEU:HB2	1.97	0.46
1:A:685:SER:HB3	1:A:708:PHE:CZ	2.51	0.46
1:A:794:ILE:N	1:A:794:ILE:HD12	2.31	0.46
1:A:842:PHE:O	1:A:842:PHE:CG	2.68	0.46
1:F:685:SER:HB3	1:F:708:PHE:CZ	2.51	0.46
1:F:857:ALA:O	1:F:860:LEU:HB2	2.16	0.46
1:F:906:MET:HB2	1:F:906:MET:HE3	1.76	0.46
1:G:685:SER:HB3	1:G:708:PHE:CZ	2.51	0.46
1:B:1095:VAL:O	1:B:1099:VAL:HG23	2.16	0.45
1:D:842:PHE:CG	1:D:842:PHE:O	2.68	0.45
1:E:1082:ASP:HA	1:E:1085:THR:HB	1.99	0.45
1:G:842:PHE:CG	1:G:842:PHE:O	2.68	0.45
1:G:1095:VAL:O	1:G:1099:VAL:HG23	2.16	0.45
1:E:672:ASN:ND2	1:E:672:ASN:H	2.13	0.45
1:E:914:LEU:O	1:E:943:CYS:HB2	2.16	0.45
1:F:794:ILE:N	1:F:794:ILE:HD12	2.32	0.45
1:F:964:ASP:HA	1:F:965:PRO:HD2	1.84	0.45
1:F:1037:LEU:C	1:F:1039:ARG:H	2.18	0.45
1:G:672:ASN:H	1:G:672:ASN:ND2	2.13	0.45
1:B:685:SER:HB3	1:B:708:PHE:CZ	2.51	0.45
1:C:857:ALA:O	1:C:860:LEU:HB2	2.16	0.45
1:D:1095:VAL:O	1:D:1099:VAL:HG23	2.17	0.45
1:E:794:ILE:N	1:E:794:ILE:HD12	2.32	0.45
1:E:1037:LEU:C	1:E:1039:ARG:H	2.18	0.45
1:F:794:ILE:O	1:F:832:CYS:HB2	2.16	0.45
1:F:805:VAL:HA	1:F:823:ARG:O	2.17	0.45
1:G:782:ALA:HA	1:G:906:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:857:ALA:O	1:G:860:LEU:HB2	2.16	0.45
1:B:1082:ASP:HA	1:B:1085:THR:HB	1.99	0.45
1:C:685:SER:HB3	1:C:708:PHE:CZ	2.51	0.45
1:C:794:ILE:O	1:C:832:CYS:HB2	2.16	0.45
1:D:1082:ASP:HA	1:D:1085:THR:HB	1.98	0.45
1:E:805:VAL:HA	1:E:823:ARG:O	2.17	0.45
1:F:687:THR:HG23	1:F:704:MET:HG2	1.98	0.45
1:F:914:LEU:O	1:F:943:CYS:HB2	2.16	0.45
1:F:1095:VAL:O	1:F:1099:VAL:HG23	2.17	0.45
1:G:794:ILE:HD12	1:G:794:ILE:N	2.31	0.45
1:G:805:VAL:HA	1:G:823:ARG:O	2.17	0.45
1:C:687:THR:HG23	1:C:704:MET:HG2	1.98	0.45
1:C:725:HIS:CG	1:C:726:PRO:HD2	2.50	0.45
1:D:794:ILE:HD12	1:D:794:ILE:N	2.32	0.45
1:E:737:THR:C	1:E:739:ARG:H	2.19	0.45
1:G:687:THR:HG23	1:G:704:MET:HG2	1.98	0.45
1:A:805:VAL:HA	1:A:823:ARG:O	2.17	0.45
1:E:685:SER:HB3	1:E:708:PHE:CZ	2.51	0.45
1:G:906:MET:HE3	1:G:906:MET:HB2	1.81	0.45
1:E:794:ILE:O	1:E:832:CYS:HB2	2.16	0.45
1:F:1082:ASP:HA	1:F:1085:THR:HB	1.98	0.45
1:A:1082:ASP:HA	1:A:1085:THR:HB	1.99	0.45
1:B:670:LEU:O	1:B:735:GLU:OE2	2.35	0.45
1:C:805:VAL:HA	1:C:823:ARG:O	2.17	0.45
1:D:841:SEP:O3P	1:E:678:LYS:NZ	2.45	0.45
1:E:1095:VAL:O	1:E:1099:VAL:HG23	2.17	0.45
1:G:670:LEU:O	1:G:735:GLU:OE2	2.35	0.45
1:A:758:SER:O	1:A:759:LYS:HB3	2.17	0.45
1:B:946:ASP:HB3	1:B:949:LEU:HD12	1.99	0.45
1:E:857:ALA:O	1:E:860:LEU:HB2	2.16	0.45
1:E:946:ASP:HB3	1:E:949:LEU:HD12	1.99	0.45
1:F:758:SER:O	1:F:759:LYS:HB3	2.17	0.45
1:A:857:ALA:O	1:A:860:LEU:HB2	2.16	0.45
1:B:794:ILE:HD12	1:B:794:ILE:N	2.32	0.45
1:E:670:LEU:O	1:E:735:GLU:OE2	2.35	0.45
1:A:670:LEU:O	1:A:735:GLU:OE2	2.35	0.44
1:B:678:LYS:HE3	1:C:841:SEP:O2P	2.17	0.44
1:C:794:ILE:N	1:C:794:ILE:HD12	2.32	0.44
1:D:792:LYS:HE2	1:D:792:LYS:HB2	1.88	0.44
1:D:805:VAL:HA	1:D:823:ARG:O	2.17	0.44
1:G:946:ASP:HB3	1:G:949:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:THR:HG23	1:A:704:MET:HG2	1.98	0.44
1:B:805:VAL:HA	1:B:823:ARG:O	2.17	0.44
1:C:792:LYS:HE2	1:C:792:LYS:HB2	1.88	0.44
1:A:946:ASP:HB3	1:A:949:LEU:HD12	1.99	0.44
1:B:758:SER:O	1:B:759:LYS:HB3	2.17	0.44
1:C:758:SER:O	1:C:759:LYS:HB3	2.17	0.44
1:F:946:ASP:HB3	1:F:949:LEU:HD12	1.99	0.44
1:G:1082:ASP:HA	1:G:1085:THR:HB	1.99	0.44
1:B:906:MET:HE3	1:B:906:MET:HB2	1.76	0.44
1:B:1033:PHE:CE1	1:B:1058:LYS:HE2	2.53	0.44
1:B:1093:ILE:HG23	1:B:1094:GLY:N	2.33	0.44
1:C:1082:ASP:HA	1:C:1085:THR:HB	1.99	0.44
1:C:1093:ILE:HG23	1:C:1094:GLY:N	2.33	0.44
1:F:1093:ILE:HG23	1:F:1094:GLY:N	2.33	0.44
1:A:1095:VAL:O	1:A:1099:VAL:HG23	2.17	0.44
1:C:1095:VAL:O	1:C:1099:VAL:HG23	2.17	0.44
1:D:670:LEU:O	1:D:735:GLU:OE2	2.35	0.44
1:D:946:ASP:HB3	1:D:949:LEU:HD12	1.99	0.44
1:E:758:SER:O	1:E:759:LYS:HB3	2.17	0.44
1:G:845:ASN:N	1:G:845:ASN:ND2	2.66	0.44
1:C:670:LEU:O	1:C:735:GLU:OE2	2.35	0.44
1:A:1093:ILE:HG23	1:A:1094:GLY:N	2.33	0.44
1:B:845:ASN:N	1:B:845:ASN:ND2	2.66	0.44
1:C:1103:LEU:C	1:C:1105:ASP:H	2.22	0.44
1:D:1033:PHE:CE1	1:D:1058:LYS:HE2	2.53	0.44
1:E:1093:ILE:HG23	1:E:1094:GLY:N	2.33	0.44
1:F:845:ASN:N	1:F:845:ASN:ND2	2.66	0.44
1:G:785:VAL:HG21	1:G:906:MET:HE3	2.00	0.44
1:G:1033:PHE:CE1	1:G:1058:LYS:HE2	2.53	0.44
1:A:798:LEU:HD23	1:A:798:LEU:HA	1.81	0.43
1:F:1033:PHE:CE1	1:F:1058:LYS:HE2	2.53	0.43
1:A:925:TYR:CD2	1:A:925:TYR:N	2.87	0.43
1:A:1103:LEU:C	1:A:1105:ASP:H	2.22	0.43
1:C:719:LEU:HD23	1:C:719:LEU:HA	1.71	0.43
1:D:767:LYS:HB2	1:D:767:LYS:HE2	1.81	0.43
1:F:670:LEU:O	1:F:735:GLU:OE2	2.35	0.43
1:F:864:SER:O	1:F:893:THR:OG1	2.29	0.43
1:F:1103:LEU:C	1:F:1105:ASP:H	2.22	0.43
1:D:1093:ILE:HG23	1:D:1094:GLY:N	2.33	0.43
1:E:925:TYR:CD2	1:E:925:TYR:N	2.87	0.43
1:E:1033:PHE:CE1	1:E:1058:LYS:HE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1103:LEU:C	1:E:1105:ASP:H	2.22	0.43
1:G:798:LEU:HD23	1:G:798:LEU:HA	1.81	0.43
1:A:729:ILE:HD12	1:A:745:LEU:HB3	2.01	0.43
1:A:761:VAL:HG11	1:F:840:SEP:O2P	2.19	0.43
1:B:925:TYR:CD2	1:B:925:TYR:N	2.87	0.43
1:C:845:ASN:N	1:C:845:ASN:ND2	2.66	0.43
1:C:946:ASP:HB3	1:C:949:LEU:HD12	1.99	0.43
1:F:925:TYR:CD2	1:F:925:TYR:N	2.87	0.43
1:G:758:SER:O	1:G:759:LYS:HB3	2.17	0.43
1:G:1093:ILE:HG23	1:G:1094:GLY:N	2.33	0.43
1:D:685:SER:HB3	1:D:708:PHE:CZ	2.51	0.43
1:G:1103:LEU:C	1:G:1105:ASP:H	2.22	0.43
1:C:1033:PHE:CE1	1:C:1058:LYS:HE2	2.53	0.43
1:D:729:ILE:HD12	1:D:745:LEU:HB3	2.01	0.43
1:E:729:ILE:HD12	1:E:745:LEU:HB3	2.01	0.43
1:G:925:TYR:CD2	1:G:925:TYR:N	2.87	0.43
1:D:758:SER:O	1:D:759:LYS:HB3	2.17	0.43
1:D:925:TYR:CD2	1:D:925:TYR:N	2.87	0.43
1:F:767:LYS:HB2	1:F:767:LYS:HE2	1.81	0.43
1:F:1108:ILE:HD11	1:G:1059:TYR:CZ	2.53	0.43
1:A:1033:PHE:CE1	1:A:1058:LYS:HE2	2.53	0.43
1:B:729:ILE:HD12	1:B:745:LEU:HB3	2.01	0.43
1:C:906:MET:HE3	1:C:906:MET:HB2	1.78	0.43
1:E:758:SER:CB	1:E:768:LEU:HD21	2.49	0.43
1:E:845:ASN:N	1:E:845:ASN:ND2	2.66	0.43
1:E:1020:ILE:HG22	1:E:1021:PRO:C	2.39	0.43
1:F:758:SER:CB	1:F:768:LEU:HD21	2.49	0.43
1:A:758:SER:CB	1:A:768:LEU:HD21	2.49	0.43
1:B:1020:ILE:HG22	1:B:1021:PRO:C	2.39	0.43
1:C:729:ILE:HD12	1:C:745:LEU:HB3	2.01	0.43
1:F:1033:PHE:CD2	1:F:1034:MET:HE3	2.54	0.43
1:B:1008:LEU:HD23	1:B:1008:LEU:HA	1.76	0.43
1:C:1020:ILE:HG22	1:C:1021:PRO:C	2.39	0.43
1:D:845:ASN:N	1:D:845:ASN:ND2	2.66	0.43
1:A:845:ASN:N	1:A:845:ASN:ND2	2.66	0.42
1:G:758:SER:CB	1:G:768:LEU:HD21	2.49	0.42
1:F:729:ILE:HD12	1:F:745:LEU:HB3	2.01	0.42
1:G:1033:PHE:CD2	1:G:1034:MET:HE3	2.54	0.42
1:D:999:ILE:N	1:D:999:ILE:HD12	2.34	0.42
1:F:694:PHE:CG	1:F:695:GLN:N	2.87	0.42
1:F:798:LEU:HD23	1:F:798:LEU:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:999:ILE:N	1:F:999:ILE:HD12	2.34	0.42
1:F:1003:ASP:HA	1:F:1004:PRO:HA	1.88	0.42
1:A:694:PHE:CG	1:A:695:GLN:N	2.87	0.42
1:B:694:PHE:CG	1:B:695:GLN:N	2.87	0.42
1:C:925:TYR:CD2	1:C:925:TYR:N	2.87	0.42
1:D:758:SER:CB	1:D:768:LEU:HD21	2.49	0.42
1:D:1103:LEU:C	1:D:1105:ASP:H	2.22	0.42
1:E:767:LYS:HB2	1:E:767:LYS:HE2	1.81	0.42
1:G:729:ILE:HD12	1:G:745:LEU:HB3	2.01	0.42
1:A:1003:ASP:HA	1:A:1004:PRO:HA	1.88	0.42
1:B:758:SER:CB	1:B:768:LEU:HD21	2.49	0.42
1:B:964:ASP:HA	1:B:965:PRO:HD2	1.84	0.42
1:C:758:SER:CB	1:C:768:LEU:HD21	2.49	0.42
1:D:810:ARG:H	1:D:810:ARG:HG3	1.68	0.42
1:E:999:ILE:HD12	1:E:999:ILE:N	2.35	0.42
1:G:999:ILE:HD12	1:G:999:ILE:N	2.35	0.42
1:A:762:SER:O	1:A:765:ASN:HB3	2.20	0.42
1:F:1020:ILE:HG22	1:F:1021:PRO:C	2.39	0.42
1:A:712:ALA:O	1:A:716:ILE:HG12	2.20	0.42
1:A:799:LYS:NZ	1:A:852:THR:HG23	2.35	0.42
1:A:906:MET:HB2	1:A:906:MET:HE3	1.76	0.42
1:C:898:THR:HG23	1:C:900:SER:OG	2.20	0.42
1:D:785:VAL:CG2	1:D:906:MET:HE1	2.50	0.42
1:E:898:THR:HG23	1:E:900:SER:OG	2.20	0.42
1:F:898:THR:HG23	1:F:900:SER:OG	2.20	0.42
1:G:719:LEU:HD23	1:G:719:LEU:HA	1.71	0.42
1:C:694:PHE:CG	1:C:695:GLN:N	2.87	0.42
1:C:799:LYS:NZ	1:C:852:THR:HG23	2.35	0.42
1:G:1020:ILE:HG22	1:G:1021:PRO:C	2.39	0.42
1:B:762:SER:O	1:B:765:ASN:HB3	2.20	0.42
1:B:999:ILE:HD12	1:B:999:ILE:N	2.34	0.42
1:B:1103:LEU:C	1:B:1105:ASP:H	2.22	0.42
1:C:712:ALA:O	1:C:716:ILE:HG12	2.20	0.42
1:C:762:SER:O	1:C:765:ASN:HB3	2.20	0.42
1:C:767:LYS:HB2	1:C:767:LYS:HE2	1.81	0.42
1:D:762:SER:O	1:D:765:ASN:HB3	2.20	0.42
1:D:798:LEU:HA	1:D:798:LEU:HD23	1.81	0.42
1:D:898:THR:HG23	1:D:900:SER:OG	2.20	0.42
1:D:1020:ILE:HG22	1:D:1021:PRO:C	2.39	0.42
1:D:1030:ASP:N	1:D:1030:ASP:OD1	2.53	0.42
1:E:799:LYS:NZ	1:E:852:THR:HG23	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:799:LYS:NZ	1:F:852:THR:HG23	2.35	0.42
1:A:787:HIS:O	1:A:790:SER:HB2	2.20	0.42
1:A:898:THR:HG23	1:A:900:SER:OG	2.20	0.42
1:A:999:ILE:N	1:A:999:ILE:HD12	2.35	0.42
1:D:1052:LEU:HD12	1:D:1052:LEU:HA	1.83	0.42
1:E:712:ALA:O	1:E:716:ILE:HG12	2.20	0.42
1:E:762:SER:O	1:E:765:ASN:HB3	2.20	0.42
1:G:799:LYS:NZ	1:G:852:THR:HG23	2.35	0.42
1:G:1030:ASP:OD1	1:G:1030:ASP:N	2.53	0.42
1:A:964:ASP:HA	1:A:965:PRO:HD2	1.84	0.41
1:A:1020:ILE:HG22	1:A:1021:PRO:C	2.39	0.41
1:A:1030:ASP:N	1:A:1030:ASP:OD1	2.53	0.41
1:C:1008:LEU:HD23	1:C:1008:LEU:HA	1.77	0.41
1:E:1033:PHE:CD2	1:E:1034:MET:HE2	2.54	0.41
1:B:725:HIS:CD2	1:B:727:ASN:HB2	2.56	0.41
1:C:999:ILE:HD12	1:C:999:ILE:N	2.35	0.41
1:D:725:HIS:CD2	1:D:727:ASN:HB2	2.55	0.41
1:E:1030:ASP:OD1	1:E:1030:ASP:N	2.53	0.41
1:G:787:HIS:O	1:G:790:SER:HB2	2.20	0.41
1:G:1106:ASP:O	1:G:1110:ARG:HG3	2.20	0.41
1:A:792:LYS:HE2	1:A:792:LYS:HB2	1.88	0.41
1:D:843:ARG:HH12	1:E:678:LYS:HD3	1.86	0.41
1:D:964:ASP:HA	1:D:965:PRO:HD2	1.84	0.41
1:E:694:PHE:CG	1:E:695:GLN:N	2.87	0.41
1:E:787:HIS:O	1:E:790:SER:HB2	2.20	0.41
1:E:1052:LEU:HD12	1:E:1052:LEU:HA	1.83	0.41
1:F:762:SER:O	1:F:765:ASN:HB3	2.20	0.41
1:F:1048:LEU:O	1:F:1049:MET:C	2.59	0.41
1:B:898:THR:HG23	1:B:900:SER:OG	2.20	0.41
1:D:712:ALA:O	1:D:716:ILE:HG12	2.20	0.41
1:E:740:PHE:HB3	1:E:741:LEU:H	1.63	0.41
1:F:787:HIS:O	1:F:790:SER:HB2	2.20	0.41
1:A:725:HIS:CD2	1:A:727:ASN:HB2	2.55	0.41
1:A:1048:LEU:O	1:A:1049:MET:C	2.59	0.41
1:D:787:HIS:O	1:D:790:SER:HB2	2.21	0.41
1:D:1067:GLU:H	1:D:1067:GLU:HG3	1.71	0.41
1:E:725:HIS:CD2	1:E:727:ASN:HB2	2.56	0.41
1:F:1106:ASP:O	1:F:1110:ARG:HG3	2.21	0.41
1:G:694:PHE:CG	1:G:695:GLN:N	2.87	0.41
1:A:785:VAL:HG21	1:A:906:MET:HE1	2.02	0.41
1:B:792:LYS:HE2	1:B:792:LYS:HB2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:799:LYS:NZ	1:B:852:THR:HG23	2.35	0.41
1:D:1020:ILE:HB	1:D:1021:PRO:HA	2.03	0.41
1:D:1106:ASP:O	1:D:1110:ARG:HG3	2.21	0.41
1:F:712:ALA:O	1:F:716:ILE:HG12	2.20	0.41
1:E:848:ASN:CB	1:E:849:PRO:HA	2.29	0.41
1:F:1020:ILE:HB	1:F:1021:PRO:HA	2.03	0.41
1:G:762:SER:O	1:G:765:ASN:HB3	2.20	0.41
1:A:811:PHE:HB3	1:A:823:ARG:HG3	2.03	0.41
1:B:1106:ASP:O	1:B:1110:ARG:HG3	2.20	0.41
1:C:787:HIS:O	1:C:790:SER:HB2	2.21	0.41
1:C:811:PHE:HB3	1:C:823:ARG:HG3	2.03	0.41
1:C:1020:ILE:HB	1:C:1021:PRO:HA	2.03	0.41
1:C:1048:LEU:O	1:C:1049:MET:C	2.59	0.41
1:E:1020:ILE:HB	1:E:1021:PRO:HA	2.03	0.41
1:F:725:HIS:CD2	1:F:727:ASN:HB2	2.56	0.41
1:G:811:PHE:HB3	1:G:823:ARG:HG3	2.03	0.41
1:A:1106:ASP:O	1:A:1110:ARG:HG3	2.21	0.41
1:B:1020:ILE:HB	1:B:1021:PRO:HA	2.03	0.41
1:C:1106:ASP:O	1:C:1110:ARG:HG3	2.20	0.41
1:D:740:PHE:HB3	1:D:741:LEU:H	1.63	0.41
1:D:799:LYS:NZ	1:D:852:THR:HG23	2.35	0.41
1:D:1048:LEU:O	1:D:1049:MET:C	2.59	0.41
1:E:811:PHE:HB3	1:E:823:ARG:HG3	2.03	0.41
1:E:1048:LEU:O	1:E:1049:MET:C	2.59	0.41
1:G:712:ALA:O	1:G:716:ILE:HG12	2.20	0.41
1:G:725:HIS:CD2	1:G:727:ASN:HB2	2.55	0.41
1:G:1020:ILE:HB	1:G:1021:PRO:HA	2.03	0.41
1:B:1030:ASP:OD1	1:B:1030:ASP:N	2.53	0.41
1:B:1055:LEU:HD23	1:B:1055:LEU:O	2.21	0.41
1:C:798:LEU:HD23	1:C:798:LEU:HA	1.80	0.41
1:C:1033:PHE:CD2	1:C:1034:MET:HE3	2.55	0.41
1:D:821:ASN:O	1:D:822:LEU:HB3	2.21	0.41
1:E:1106:ASP:O	1:E:1110:ARG:HG3	2.20	0.41
1:G:773:ASN:HA	1:G:774:PRO:HD2	1.92	0.41
1:G:898:THR:HG23	1:G:900:SER:OG	2.20	0.41
1:G:915:SER:HB2	1:G:918:LYS:HB2	2.03	0.41
1:B:811:PHE:HB3	1:B:823:ARG:HG3	2.03	0.40
1:B:924:LYS:HG3	1:B:925:TYR:HD2	1.87	0.40
1:C:898:THR:OG1	1:C:899:ARG:N	2.55	0.40
1:C:1108:ILE:HD11	1:D:1059:TYR:OH	2.21	0.40
1:E:785:VAL:HG21	1:E:906:MET:CE	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:821:ASN:O	1:E:822:LEU:HB3	2.22	0.40
1:E:1055:LEU:HD23	1:E:1055:LEU:O	2.21	0.40
1:F:968:ARG:HA	1:F:969:PRO:HD2	1.92	0.40
1:A:785:VAL:HG21	1:A:906:MET:CE	2.52	0.40
1:A:821:ASN:O	1:A:822:LEU:HB3	2.22	0.40
1:A:898:THR:OG1	1:A:899:ARG:N	2.54	0.40
1:A:1020:ILE:HB	1:A:1021:PRO:HA	2.03	0.40
1:B:737:THR:HG23	1:B:740:PHE:N	2.37	0.40
1:B:740:PHE:HB3	1:B:741:LEU:H	1.63	0.40
1:B:785:VAL:HG21	1:B:906:MET:CE	2.52	0.40
1:C:725:HIS:CD2	1:C:727:ASN:HB2	2.55	0.40
1:C:1030:ASP:OD1	1:C:1030:ASP:N	2.53	0.40
1:D:785:VAL:HG21	1:D:906:MET:CE	2.51	0.40
1:D:811:PHE:HB3	1:D:823:ARG:HG3	2.03	0.40
1:E:915:SER:HB2	1:E:918:LYS:HB2	2.04	0.40
1:F:785:VAL:HG21	1:F:906:MET:CE	2.52	0.40
1:F:1030:ASP:OD1	1:F:1030:ASP:N	2.53	0.40
1:G:785:VAL:HG21	1:G:906:MET:CE	2.51	0.40
1:A:924:LYS:HG3	1:A:925:TYR:HD2	1.86	0.40
1:B:712:ALA:O	1:B:716:ILE:HG12	2.20	0.40
1:B:787:HIS:O	1:B:790:SER:HB2	2.20	0.40
1:B:821:ASN:O	1:B:822:LEU:HB3	2.21	0.40
1:B:840:SEP:O2P	1:G:761:VAL:HG11	2.20	0.40
1:B:1048:LEU:O	1:B:1049:MET:C	2.59	0.40
1:D:737:THR:HG23	1:D:740:PHE:N	2.36	0.40
1:D:1055:LEU:HD23	1:D:1055:LEU:O	2.21	0.40
1:F:915:SER:HB2	1:F:918:LYS:HB2	2.03	0.40
1:A:705:LEU:HD12	1:A:705:LEU:N	2.37	0.40
1:B:915:SER:HB2	1:B:918:LYS:HB2	2.03	0.40
1:C:821:ASN:O	1:C:822:LEU:HB3	2.21	0.40
1:E:898:THR:OG1	1:E:899:ARG:N	2.54	0.40
1:E:1008:LEU:HD23	1:E:1008:LEU:HA	1.76	0.40
1:A:1011:LYS:HE2	1:A:1011:LYS:HA	2.04	0.40
1:A:1055:LEU:HD23	1:A:1055:LEU:O	2.21	0.40
1:C:1055:LEU:HD23	1:C:1055:LEU:O	2.21	0.40
1:E:1088:PHE:HA	1:E:1089:PRO:HD2	1.93	0.40
1:F:898:THR:OG1	1:F:899:ARG:N	2.55	0.40
1:F:1055:LEU:HD23	1:F:1055:LEU:O	2.21	0.40
1:G:705:LEU:N	1:G:705:LEU:HD12	2.37	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1003:ASP:O	1:E:1042:LYS:NZ[4_555]	1.44	0.76
1:E:1003:ASP:O	1:E:1042:LYS:CE[4_555]	1.50	0.70
1:E:1003:ASP:C	1:E:1042:LYS:NZ[4_555]	1.70	0.50
1:E:1003:ASP:OD2	1:E:1044:HIS:NE2[4_555]	1.73	0.47
1:C:761:VAL:CG1	1:E:840:SEP:O2P[2_555]	1.96	0.24
1:E:1003:ASP:OD2	1:E:1044:HIS:CD2[4_555]	2.07	0.13
1:E:1059:TYR:OH	1:E:1108:ILE:CD1[2_555]	2.12	0.08

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	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6 35
1	B	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6 35
1	C	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6 35
1	D	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6 35
1	E	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6 35
1	F	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6 35
1	G	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6 35
All	All	2891/3136 (92%)	2464 (85%)	364 (13%)	63 (2%)	6 35

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	759	LYS
1	A	770	LYS
1	A	771	GLU
1	A	862	GLU
1	B	759	LYS
1	B	770	LYS
1	B	771	GLU

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Mol	Chain	Res	Type
1	B	862	GLU
1	C	759	LYS
1	C	770	LYS
1	C	771	GLU
1	C	862	GLU
1	D	759	LYS
1	D	770	LYS
1	D	771	GLU
1	D	862	GLU
1	E	759	LYS
1	E	770	LYS
1	E	771	GLU
1	E	862	GLU
1	F	759	LYS
1	F	770	LYS
1	F	771	GLU
1	F	862	GLU
1	G	759	LYS
1	G	770	LYS
1	G	771	GLU
1	G	862	GLU
1	A	893	THR
1	B	893	THR
1	C	893	THR
1	D	893	THR
1	E	893	THR
1	F	893	THR
1	G	893	THR
1	A	1104	SER
1	B	1104	SER
1	C	1104	SER
1	D	1104	SER
1	E	1104	SER
1	F	1104	SER
1	G	1104	SER
1	A	738	ASP
1	B	738	ASP
1	C	738	ASP
1	D	738	ASP
1	E	738	ASP
1	F	738	ASP
1	G	738	ASP

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Mol	Chain	Res	Type
1	A	838	GLY
1	B	838	GLY
1	C	838	GLY
1	D	838	GLY
1	E	838	GLY
1	F	838	GLY
1	G	838	GLY
1	A	849	PRO
1	B	849	PRO
1	C	849	PRO
1	D	849	PRO
1	E	849	PRO
1	F	849	PRO
1	G	849	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/405 (94%)	352 (93%)	28 (7%)	13	38
1	B	380/405 (94%)	352 (93%)	28 (7%)	13	38
1	C	380/405 (94%)	352 (93%)	28 (7%)	13	38
1	D	380/405 (94%)	352 (93%)	28 (7%)	13	38
1	E	380/405 (94%)	352 (93%)	28 (7%)	13	38
1	F	380/405 (94%)	352 (93%)	28 (7%)	13	38
1	G	380/405 (94%)	352 (93%)	28 (7%)	13	38
All	All	2660/2835 (94%)	2464 (93%)	196 (7%)	13	38

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	670	LEU
1	A	671	LYS
1	A	672	ASN

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Mol	Chain	Res	Type
1	A	707	ASP
1	A	711	ILE
1	A	729	ILE
1	A	749	ASN
1	A	750	LEU
1	A	759	LYS
1	A	761	VAL
1	A	767	LYS
1	A	788	LEU
1	A	796	ARG
1	A	804	LEU
1	A	817	THR
1	A	823	ARG
1	A	835	LEU
1	A	843	ARG
1	A	845	ASN
1	A	939	ASP
1	A	943	CYS
1	A	970	THR
1	A	987	LEU
1	A	1030	ASP
1	A	1040	TYR
1	A	1053	ARG
1	A	1067	GLU
1	A	1085	THR
1	B	670	LEU
1	B	671	LYS
1	B	672	ASN
1	B	707	ASP
1	B	711	ILE
1	B	729	ILE
1	B	749	ASN
1	B	750	LEU
1	B	759	LYS
1	B	761	VAL
1	B	767	LYS
1	B	788	LEU
1	B	796	ARG
1	B	804	LEU
1	B	817	THR
1	B	823	ARG
1	B	835	LEU

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Mol	Chain	Res	Type
1	B	843	ARG
1	B	845	ASN
1	B	939	ASP
1	B	943	CYS
1	B	970	THR
1	B	987	LEU
1	B	1030	ASP
1	B	1040	TYR
1	B	1053	ARG
1	B	1067	GLU
1	B	1085	THR
1	C	670	LEU
1	C	671	LYS
1	C	672	ASN
1	C	707	ASP
1	C	711	ILE
1	C	729	ILE
1	C	749	ASN
1	C	750	LEU
1	C	759	LYS
1	C	761	VAL
1	C	767	LYS
1	C	788	LEU
1	C	796	ARG
1	C	804	LEU
1	C	817	THR
1	C	823	ARG
1	C	835	LEU
1	C	843	ARG
1	C	845	ASN
1	C	939	ASP
1	C	943	CYS
1	C	970	THR
1	C	987	LEU
1	C	1030	ASP
1	C	1040	TYR
1	C	1053	ARG
1	C	1067	GLU
1	C	1085	THR
1	D	670	LEU
1	D	671	LYS
1	D	672	ASN

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Mol	Chain	Res	Type
1	D	707	ASP
1	D	711	ILE
1	D	729	ILE
1	D	749	ASN
1	D	750	LEU
1	D	759	LYS
1	D	761	VAL
1	D	767	LYS
1	D	788	LEU
1	D	796	ARG
1	D	804	LEU
1	D	817	THR
1	D	823	ARG
1	D	835	LEU
1	D	843	ARG
1	D	845	ASN
1	D	939	ASP
1	D	943	CYS
1	D	970	THR
1	D	987	LEU
1	D	1030	ASP
1	D	1040	TYR
1	D	1053	ARG
1	D	1067	GLU
1	D	1085	THR
1	E	670	LEU
1	E	671	LYS
1	E	672	ASN
1	E	707	ASP
1	E	711	ILE
1	E	729	ILE
1	E	749	ASN
1	E	750	LEU
1	E	759	LYS
1	E	761	VAL
1	E	767	LYS
1	E	788	LEU
1	E	796	ARG
1	E	804	LEU
1	E	817	THR
1	E	823	ARG
1	E	835	LEU

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Mol	Chain	Res	Type
1	E	843	ARG
1	E	845	ASN
1	E	939	ASP
1	E	943	CYS
1	E	970	THR
1	E	987	LEU
1	E	1030	ASP
1	E	1040	TYR
1	E	1053	ARG
1	E	1067	GLU
1	E	1085	THR
1	F	670	LEU
1	F	671	LYS
1	F	672	ASN
1	F	707	ASP
1	F	711	ILE
1	F	729	ILE
1	F	749	ASN
1	F	750	LEU
1	F	759	LYS
1	F	761	VAL
1	F	767	LYS
1	F	788	LEU
1	F	796	ARG
1	F	804	LEU
1	F	817	THR
1	F	823	ARG
1	F	835	LEU
1	F	843	ARG
1	F	845	ASN
1	F	939	ASP
1	F	943	CYS
1	F	970	THR
1	F	987	LEU
1	F	1030	ASP
1	F	1040	TYR
1	F	1053	ARG
1	F	1067	GLU
1	F	1085	THR
1	G	670	LEU
1	G	671	LYS
1	G	672	ASN

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Mol	Chain	Res	Type
1	G	707	ASP
1	G	711	ILE
1	G	729	ILE
1	G	749	ASN
1	G	750	LEU
1	G	759	LYS
1	G	761	VAL
1	G	767	LYS
1	G	788	LEU
1	G	796	ARG
1	G	804	LEU
1	G	817	THR
1	G	823	ARG
1	G	835	LEU
1	G	843	ARG
1	G	845	ASN
1	G	939	ASP
1	G	943	CYS
1	G	970	THR
1	G	987	LEU
1	G	1030	ASP
1	G	1040	TYR
1	G	1053	ARG
1	G	1067	GLU
1	G	1085	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	672	ASN
1	A	691	GLN
1	A	725	HIS
1	A	753	GLN
1	A	802	ASN
1	A	839	GLN
1	A	845	ASN
1	A	1001	ASN
1	A	1090	ASN
1	B	672	ASN
1	B	691	GLN
1	B	725	HIS
1	B	753	GLN

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Mol	Chain	Res	Type
1	B	787	HIS
1	B	802	ASN
1	B	839	GLN
1	B	845	ASN
1	B	1001	ASN
1	B	1090	ASN
1	C	672	ASN
1	C	691	GLN
1	C	725	HIS
1	C	753	GLN
1	C	802	ASN
1	C	845	ASN
1	C	1001	ASN
1	C	1090	ASN
1	D	672	ASN
1	D	725	HIS
1	D	753	GLN
1	D	802	ASN
1	D	845	ASN
1	D	1001	ASN
1	D	1090	ASN
1	E	672	ASN
1	E	691	GLN
1	E	725	HIS
1	E	753	GLN
1	E	802	ASN
1	E	839	GLN
1	E	845	ASN
1	E	1001	ASN
1	E	1090	ASN
1	F	672	ASN
1	F	691	GLN
1	F	725	HIS
1	F	753	GLN
1	F	787	HIS
1	F	802	ASN
1	F	839	GLN
1	F	845	ASN
1	F	1001	ASN
1	F	1090	ASN
1	G	672	ASN
1	G	691	GLN

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Mol	Chain	Res	Type
1	G	725	HIS
1	G	753	GLN
1	G	802	ASN
1	G	839	GLN
1	G	845	ASN
1	G	1001	ASN
1	G	1090	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

21 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	B	841	1	8,9,10	1.58	1 (12%)	7,12,14	0.74	0
1	SEP	C	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.74	0
1	SEP	D	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	TPO	F	844	1	8,10,11	3.12	5 (62%)	10,14,16	1.64	2 (20%)
1	SEP	B	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.42	1 (14%)
1	SEP	A	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	TPO	C	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	TPO	D	844	1	8,10,11	3.10	5 (62%)	10,14,16	1.65	2 (20%)
1	TPO	B	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	SEP	G	841	1	8,9,10	1.58	1 (12%)	7,12,14	0.74	0
1	SEP	D	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.41	1 (14%)
1	TPO	A	844	1	8,10,11	3.10	5 (62%)	10,14,16	1.64	2 (20%)
1	TPO	G	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	C	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.40	1 (14%)
1	SEP	F	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.41	1 (14%)
1	SEP	A	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.42	1 (14%)
1	SEP	F	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	SEP	E	841	1	8,9,10	1.58	1 (12%)	7,12,14	0.73	0
1	SEP	E	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.40	1 (14%)
1	SEP	G	840	1	8,9,10	1.65	1 (12%)	7,12,14	1.39	1 (14%)
1	TPO	E	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	841	1	-	1/6/8/10	-
1	SEP	C	841	1	-	1/6/8/10	-
1	SEP	D	841	1	-	1/6/8/10	-
1	TPO	F	844	1	-	4/9/11/13	-
1	SEP	B	840	1	-	4/6/8/10	-
1	SEP	A	841	1	-	1/6/8/10	-
1	TPO	C	844	1	-	4/9/11/13	-
1	TPO	D	844	1	-	4/9/11/13	-
1	TPO	B	844	1	-	4/9/11/13	-
1	SEP	G	841	1	-	1/6/8/10	-
1	SEP	D	840	1	-	4/6/8/10	-
1	TPO	A	844	1	-	4/9/11/13	-
1	TPO	G	844	1	-	4/9/11/13	-
1	SEP	C	840	1	-	4/6/8/10	-
1	SEP	F	840	1	-	4/6/8/10	-
1	SEP	A	840	1	-	4/6/8/10	-
1	SEP	F	841	1	-	1/6/8/10	-
1	SEP	E	841	1	-	1/6/8/10	-
1	SEP	E	840	1	-	4/6/8/10	-
1	SEP	G	840	1	-	4/6/8/10	-
1	TPO	E	844	1	-	4/9/11/13	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	844	TPO	O-C	5.56	1.41	1.20
1	D	844	TPO	O-C	5.56	1.41	1.20
1	G	844	TPO	O-C	5.56	1.41	1.20
1	C	844	TPO	O-C	5.55	1.41	1.20
1	F	844	TPO	O-C	5.55	1.41	1.20
1	A	844	TPO	O-C	5.55	1.41	1.20
1	E	844	TPO	O-C	5.55	1.41	1.20
1	F	844	TPO	P-O1P	4.73	1.65	1.50
1	D	844	TPO	P-O1P	4.73	1.65	1.50
1	E	844	TPO	P-O1P	4.73	1.65	1.50
1	A	844	TPO	P-O1P	4.72	1.65	1.50
1	C	844	TPO	P-O1P	4.72	1.65	1.50
1	B	844	TPO	P-O1P	4.72	1.65	1.50
1	G	844	TPO	P-O1P	4.71	1.65	1.50
1	B	840	SEP	P-O1P	3.63	1.61	1.50
1	G	840	SEP	P-O1P	3.62	1.61	1.50
1	F	840	SEP	P-O1P	3.62	1.61	1.50
1	C	840	SEP	P-O1P	3.60	1.61	1.50
1	D	840	SEP	P-O1P	3.60	1.61	1.50
1	E	840	SEP	P-O1P	3.60	1.61	1.50
1	A	840	SEP	P-O1P	3.59	1.61	1.50
1	G	841	SEP	P-O1P	3.46	1.61	1.50
1	E	841	SEP	P-O1P	3.45	1.61	1.50
1	C	841	SEP	P-O1P	3.45	1.61	1.50
1	B	841	SEP	P-O1P	3.45	1.61	1.50
1	A	841	SEP	P-O1P	3.43	1.61	1.50
1	F	841	SEP	P-O1P	3.42	1.61	1.50
1	D	841	SEP	P-O1P	3.42	1.61	1.50
1	F	844	TPO	P-OG1	3.36	1.65	1.59
1	B	844	TPO	P-OG1	3.35	1.65	1.59
1	E	844	TPO	P-OG1	3.33	1.65	1.59
1	G	844	TPO	P-OG1	3.31	1.65	1.59
1	C	844	TPO	P-OG1	3.30	1.65	1.59
1	A	844	TPO	P-OG1	3.29	1.65	1.59
1	D	844	TPO	P-OG1	3.29	1.65	1.59
1	C	844	TPO	P-O2P	2.68	1.64	1.54
1	B	844	TPO	P-O2P	2.67	1.64	1.54
1	G	844	TPO	P-O2P	2.67	1.64	1.54
1	E	844	TPO	P-O2P	2.66	1.64	1.54
1	A	844	TPO	P-O2P	2.66	1.64	1.54
1	F	844	TPO	P-O2P	2.66	1.64	1.54
1	D	844	TPO	P-O2P	2.65	1.64	1.54
1	C	844	TPO	P-O3P	-2.25	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	844	TPO	P-O3P	-2.25	1.46	1.54
1	B	844	TPO	P-O3P	-2.24	1.46	1.54
1	E	844	TPO	P-O3P	-2.24	1.46	1.54
1	G	844	TPO	P-O3P	-2.23	1.46	1.54
1	A	844	TPO	P-O3P	-2.23	1.46	1.54
1	D	844	TPO	P-O3P	-2.22	1.46	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	844	TPO	O-C-CA	-4.04	114.39	124.77
1	D	844	TPO	O-C-CA	-4.04	114.39	124.77
1	E	844	TPO	O-C-CA	-4.02	114.43	124.77
1	C	844	TPO	O-C-CA	-4.02	114.43	124.77
1	F	844	TPO	O-C-CA	-4.01	114.45	124.77
1	B	844	TPO	O-C-CA	-4.01	114.45	124.77
1	G	844	TPO	O-C-CA	-4.01	114.45	124.77
1	A	840	SEP	OG-CB-CA	3.38	111.43	108.14
1	B	840	SEP	OG-CB-CA	3.36	111.41	108.14
1	F	840	SEP	OG-CB-CA	3.35	111.41	108.14
1	D	840	SEP	OG-CB-CA	3.34	111.39	108.14
1	E	840	SEP	OG-CB-CA	3.31	111.37	108.14
1	C	840	SEP	OG-CB-CA	3.30	111.36	108.14
1	G	840	SEP	OG-CB-CA	3.27	111.32	108.14
1	D	844	TPO	CG2-CB-CA	-2.29	108.79	113.26
1	F	844	TPO	CG2-CB-CA	-2.28	108.81	113.26
1	G	844	TPO	CG2-CB-CA	-2.28	108.81	113.26
1	E	844	TPO	CG2-CB-CA	-2.28	108.82	113.26
1	B	844	TPO	CG2-CB-CA	-2.28	108.83	113.26
1	A	844	TPO	CG2-CB-CA	-2.27	108.83	113.26
1	C	844	TPO	CG2-CB-CA	-2.27	108.84	113.26

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	840	SEP	N-CA-CB-OG
1	A	840	SEP	CB-OG-P-O2P
1	A	840	SEP	CB-OG-P-O3P
1	A	844	TPO	N-CA-CB-CG2
1	A	844	TPO	N-CA-CB-OG1
1	A	844	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	B	840	SEP	N-CA-CB-OG
1	B	840	SEP	CB-OG-P-O2P
1	B	840	SEP	CB-OG-P-O3P
1	B	844	TPO	N-CA-CB-CG2
1	B	844	TPO	N-CA-CB-OG1
1	B	844	TPO	O-C-CA-CB
1	C	840	SEP	N-CA-CB-OG
1	C	840	SEP	CB-OG-P-O2P
1	C	840	SEP	CB-OG-P-O3P
1	C	844	TPO	N-CA-CB-CG2
1	C	844	TPO	N-CA-CB-OG1
1	C	844	TPO	O-C-CA-CB
1	D	840	SEP	N-CA-CB-OG
1	D	840	SEP	CB-OG-P-O2P
1	D	840	SEP	CB-OG-P-O3P
1	D	844	TPO	N-CA-CB-CG2
1	D	844	TPO	N-CA-CB-OG1
1	D	844	TPO	O-C-CA-CB
1	E	840	SEP	N-CA-CB-OG
1	E	840	SEP	CB-OG-P-O2P
1	E	840	SEP	CB-OG-P-O3P
1	E	844	TPO	N-CA-CB-CG2
1	E	844	TPO	N-CA-CB-OG1
1	E	844	TPO	O-C-CA-CB
1	F	840	SEP	N-CA-CB-OG
1	F	840	SEP	CB-OG-P-O2P
1	F	840	SEP	CB-OG-P-O3P
1	F	844	TPO	N-CA-CB-CG2
1	F	844	TPO	N-CA-CB-OG1
1	F	844	TPO	O-C-CA-CB
1	G	840	SEP	N-CA-CB-OG
1	G	840	SEP	CB-OG-P-O2P
1	G	840	SEP	CB-OG-P-O3P
1	G	844	TPO	N-CA-CB-CG2
1	G	844	TPO	N-CA-CB-OG1
1	G	844	TPO	O-C-CA-CB
1	A	841	SEP	CB-OG-P-O3P
1	B	841	SEP	CB-OG-P-O3P
1	C	841	SEP	CB-OG-P-O3P
1	D	841	SEP	CB-OG-P-O3P
1	E	841	SEP	CB-OG-P-O3P
1	F	841	SEP	CB-OG-P-O3P

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Mol	Chain	Res	Type	Atoms
1	G	841	SEP	CB-OG-P-O3P
1	A	844	TPO	CB-OG1-P-O1P
1	B	844	TPO	CB-OG1-P-O1P
1	C	844	TPO	CB-OG1-P-O1P
1	D	844	TPO	CB-OG1-P-O1P
1	E	844	TPO	CB-OG1-P-O1P
1	F	844	TPO	CB-OG1-P-O1P
1	G	844	TPO	CB-OG1-P-O1P
1	A	840	SEP	CB-OG-P-O1P
1	B	840	SEP	CB-OG-P-O1P
1	C	840	SEP	CB-OG-P-O1P
1	D	840	SEP	CB-OG-P-O1P
1	E	840	SEP	CB-OG-P-O1P
1	F	840	SEP	CB-OG-P-O1P
1	G	840	SEP	CB-OG-P-O1P

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	841	SEP	1	0
1	D	841	SEP	2	0
1	B	840	SEP	1	0
1	D	840	SEP	3	0
1	C	840	SEP	1	0
1	F	840	SEP	1	0
1	A	840	SEP	1	0
1	E	840	SEP	0	1

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	415/448 (92%)	0.42	39 (9%)	8	11	53, 108, 202, 287	0
1	B	415/448 (92%)	0.14	19 (4%)	32	30	53, 108, 202, 287	0
1	C	415/448 (92%)	0.04	17 (4%)	37	34	53, 108, 202, 287	0
1	D	415/448 (92%)	0.07	16 (3%)	39	34	53, 108, 202, 287	0
1	E	415/448 (92%)	0.06	11 (2%)	54	47	53, 108, 202, 287	0
1	F	415/448 (92%)	0.09	5 (1%)	79	71	53, 108, 202, 287	0
1	G	415/448 (92%)	0.14	13 (3%)	49	42	53, 108, 202, 287	0
All	All	2905/3136 (92%)	0.14	120 (4%)	37	34	53, 108, 203, 287	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	864	SER	8.4
1	A	893	THR	8.3
1	A	863	GLU	6.1
1	A	894	LYS	5.3
1	B	743	ILE	5.2
1	B	670	LEU	5.0
1	C	735	GLU	5.0
1	A	743	ILE	4.9
1	B	742	TYR	4.9
1	C	736	THR	4.8
1	B	735	GLU	4.6
1	A	734	SER	4.5
1	C	737	THR	4.4
1	A	731	TYR	4.4
1	B	734	SER	4.3
1	D	1113	LEU	4.3
1	C	742	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	746	GLU	3.8
1	C	893	THR	3.8
1	B	733	CYS	3.8
1	A	744	ALA	3.7
1	B	724	ASP	3.5
1	C	672	ASN	3.5
1	B	673	LEU	3.5
1	C	734	SER	3.5
1	C	670	LEU	3.5
1	A	733	CYS	3.4
1	E	738	ASP	3.4
1	A	735	GLU	3.4
1	A	858	PRO	3.3
1	A	746	GLU	3.3
1	A	854	GLY	3.3
1	F	734	SER	3.3
1	A	961	ILE	3.3
1	G	742	TYR	3.2
1	A	729	ILE	3.1
1	B	744	ALA	3.1
1	E	743	ILE	3.1
1	G	834	LYS	3.1
1	E	746	GLU	3.0
1	A	719	LEU	3.0
1	G	721	GLU	3.0
1	B	736	THR	3.0
1	G	743	ILE	2.9
1	A	732	TYR	2.9
1	E	739	ARG	2.9
1	C	738	ASP	2.9
1	A	742	TYR	2.9
1	G	722	SER	2.9
1	D	941	MET	2.8
1	D	893	THR	2.8
1	B	737	THR	2.8
1	D	1092	LEU	2.7
1	A	672	ASN	2.7
1	E	938	LEU	2.7
1	B	721	GLU	2.7
1	C	1113	LEU	2.7
1	A	785	VAL	2.6
1	E	734	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	919	HIS	2.6
1	A	673	LEU	2.6
1	E	737	THR	2.6
1	D	863	GLU	2.6
1	D	938	LEU	2.6
1	G	833	LYS	2.6
1	B	1091	LEU	2.6
1	B	722	SER	2.5
1	G	718	LEU	2.5
1	A	694	PHE	2.5
1	F	672	ASN	2.5
1	A	917	GLY	2.5
1	D	1012	PHE	2.4
1	C	706	ILE	2.4
1	F	743	ILE	2.4
1	D	1096	TYR	2.4
1	C	894	LYS	2.4
1	D	957	ILE	2.4
1	A	810	ARG	2.4
1	F	735	GLU	2.4
1	A	811	PHE	2.4
1	G	673	LEU	2.4
1	A	826	ILE	2.4
1	A	895	ARG	2.3
1	B	672	ASN	2.3
1	A	829	PHE	2.3
1	G	829	PHE	2.3
1	B	745	LEU	2.3
1	A	862	GLU	2.3
1	A	730	ARG	2.3
1	A	957	ILE	2.3
1	D	1095	VAL	2.3
1	D	954	THR	2.3
1	B	701	VAL	2.2
1	A	857	ALA	2.2
1	C	673	LEU	2.2
1	A	859	GLU	2.2
1	D	847	ASN	2.2
1	F	670	LEU	2.2
1	D	1091	LEU	2.2
1	A	855	TRP	2.2
1	C	1096	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	772	TYR	2.1
1	A	822	LEU	2.1
1	E	742	TYR	2.1
1	A	1039	ARG	2.1
1	D	1114	TYR	2.1
1	B	785	VAL	2.1
1	E	1049	MET	2.1
1	E	1092	LEU	2.1
1	G	734	SER	2.1
1	E	1096	TYR	2.1
1	G	731	TYR	2.1
1	G	735	GLU	2.1
1	C	709	CYS	2.0
1	A	748	CYS	2.0
1	D	856	ARG	2.0
1	C	1099	VAL	2.0
1	D	913	ILE	2.0
1	C	741	LEU	2.0
1	G	744	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	D	844	11/12	0.51	0.42	166,194,212,216	0
1	TPO	B	844	11/12	0.64	0.32	166,194,212,216	0
1	TPO	C	844	11/12	0.66	0.39	166,194,212,216	0
1	SEP	E	841	10/11	0.68	0.17	111,133,156,162	0
1	SEP	C	840	10/11	0.69	0.23	147,153,162,164	0
1	SEP	A	840	10/11	0.69	0.28	147,153,162,164	0
1	SEP	E	840	10/11	0.70	0.23	147,153,162,164	0
1	SEP	B	841	10/11	0.73	0.17	111,133,156,162	0
1	SEP	F	840	10/11	0.73	0.27	147,153,162,164	0
1	SEP	D	841	10/11	0.74	0.18	111,133,156,162	0
1	TPO	E	844	11/12	0.75	0.22	166,194,212,216	0
1	TPO	G	844	11/12	0.75	0.22	166,194,212,216	0
1	SEP	D	840	10/11	0.76	0.19	147,153,162,164	0
1	SEP	F	841	10/11	0.77	0.24	111,133,156,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	G	841	10/11	0.78	0.16	111,133,156,162	0
1	TPO	F	844	11/12	0.78	0.27	166,194,212,216	0
1	SEP	B	840	10/11	0.79	0.26	147,153,162,164	0
1	TPO	A	844	11/12	0.80	0.28	166,194,212,216	0
1	SEP	G	840	10/11	0.80	0.20	147,153,162,164	0
1	SEP	A	841	10/11	0.82	0.17	111,133,156,162	0
1	SEP	C	841	10/11	0.84	0.21	111,133,156,162	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.