



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:16 PM UTC

PDB ID : 3SDM / pdb_00003sdm
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

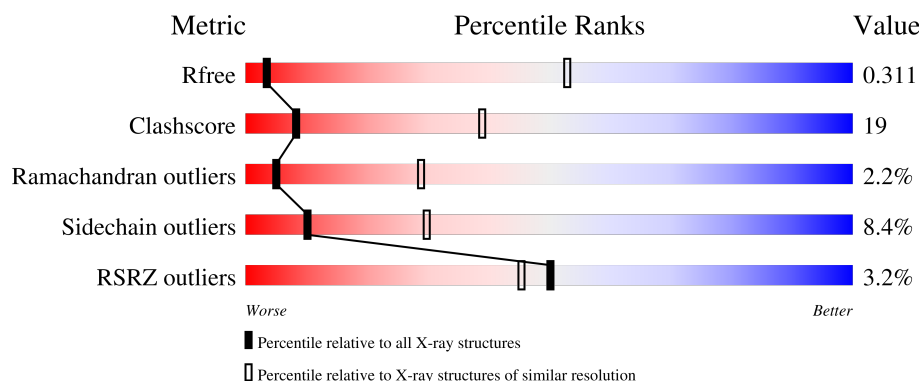
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1162 (9.00-4.00)
Clashscore	190562	1000 (9.00-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	
1	B	448	
1	C	448	
1	D	448	
1	E	448	

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Mol	Chain	Length	Quality of chain
1	F	448	2% 55% 32% 6% 7%
1	G	448	3% 55% 32% 6% 7%

2 Entry composition

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
1	A	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	B	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	C	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	D	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	E	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	F	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	G	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			

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
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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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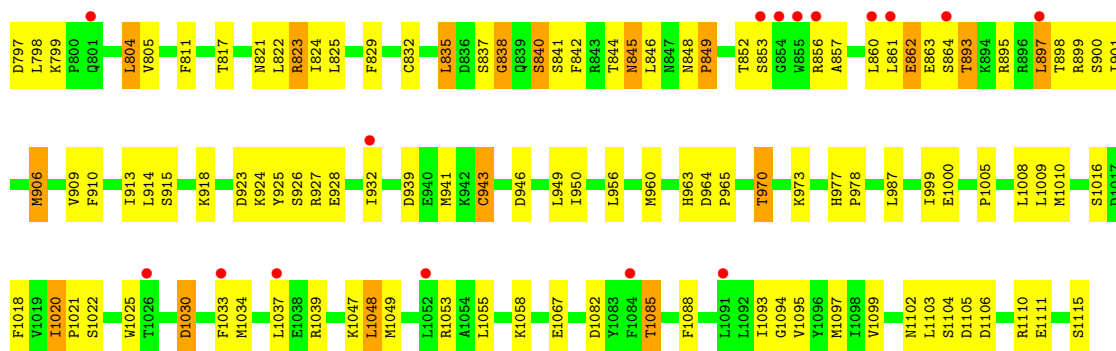
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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	TYR	deletion	UNP P32361
E	?	-	ASP	deletion	UNP P32361
E	?	-	PRO	deletion	UNP P32361
E	?	-	PHE	deletion	UNP P32361
F	640	PRO	-	expression tag	UNP P32361
F	?	-	ASN	deletion	UNP P32361
F	?	-	ASN	deletion	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

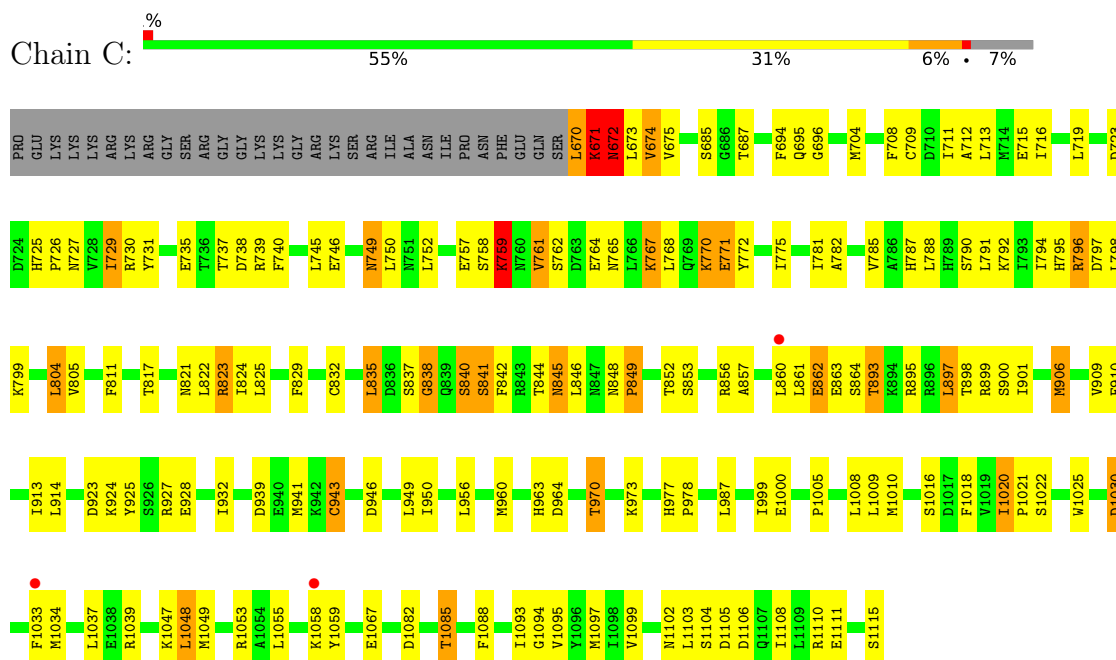
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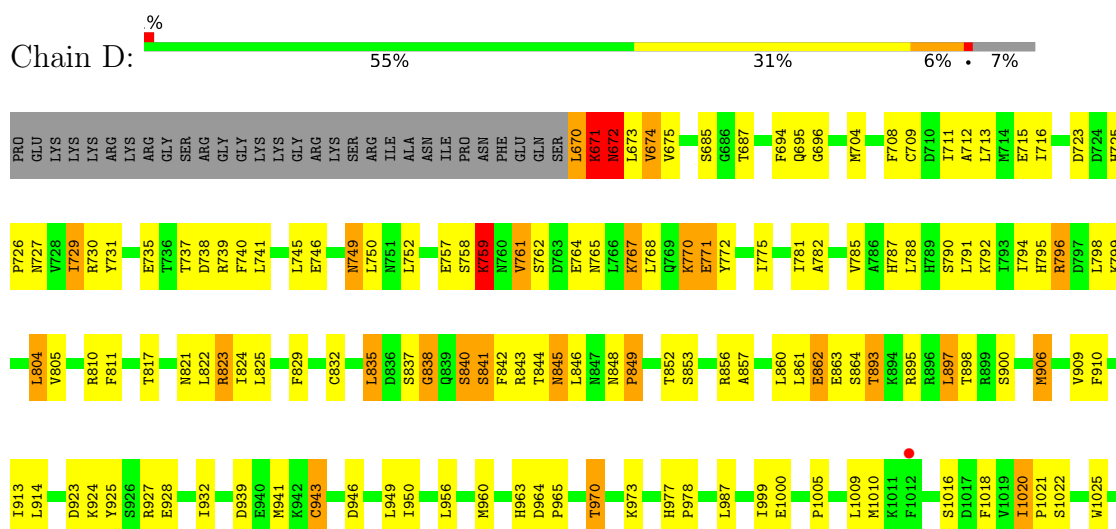
Chain	Residue	Modelled	Actual	Comment	Reference
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G	?	-	GLU	deletion	UNP P32361
G	?	-	HIS	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	ARG	deletion	UNP P32361
G	?	-	HIS	deletion	UNP 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

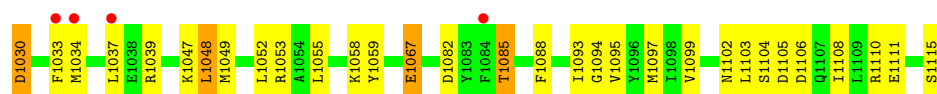


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

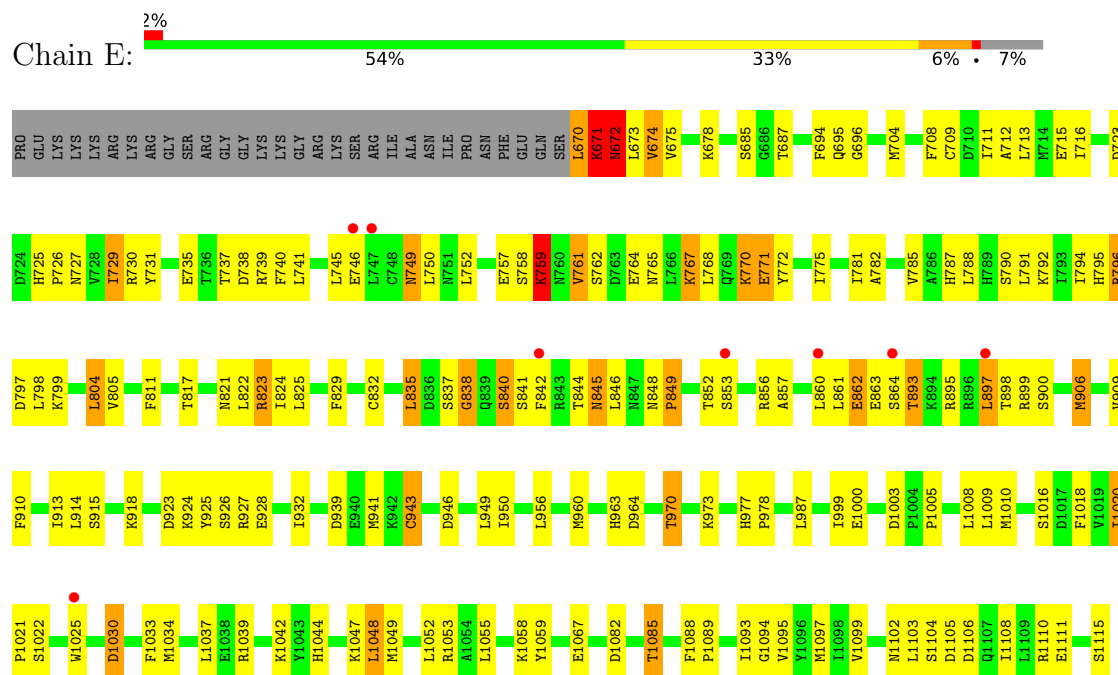


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

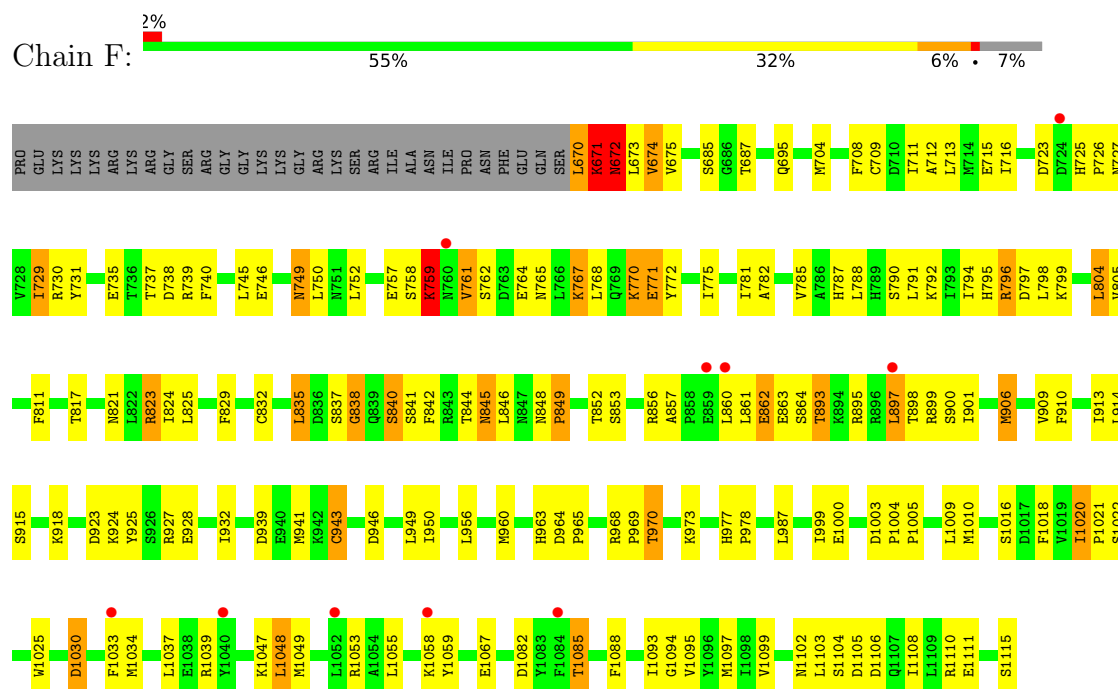




- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



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



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



PRO	GLU	LYS	LYS	LYS	ARG	LYS	ARG	GLY	SER	ARG	GLY	LYS	LYS	LYS	ARG	LYS	SER	ARG	ILE	ALA	ASN	ILE	PRO	ASN	PHE	GLU	GLN	SER	L670	K671	K672	L673	V674	V675	S685	G686	T687	F694	Q695	M704	L705	F708	C709	D710	I711	A712	L713	M714	E715	I716	L719	D723	
D724	H725	P726	N727	V728	I729	R730	Y731	E735	T736	T737	D738	R739	F740	L745	E746	N749	L750	M751	L752	E757	S758	K759	M760	V761	S762	D763	E764	N765	L766	K767	L768	Q769	K770	E771	Y772	N773	P774	I775	I781	A782	V785	A786	H787	L788	H789	S790	L791	K792	I793	I794	H795	R796	D797
L798	K799	L804	V805	F811	T817	N821	L822	R823	I824	L825	F829	C832	L835	D836	S837	G838	Q839	S840	S841	F842	R843	T844	N845	L846	R847	N848	P849	T852	S853	R856	A857	L860	L861	E862	E863	S864	T893	R894	R895	R896	L897	T898	R899	S900	I901	M906	Y909						
F910	I913	L914	S915	K918	D923	K924	Y925	S926	R927	E928	I932	D939	F940	M941	K942	C943	D946	L949	I950	L956	M960	H963	D964	P965	L966	T970	K973	H977	P978	L987	I999	E1000	P1005	L1009	M1010	S1016	D1017	F1018	V1019	I1020	P1021												
S1022	W1025	F1029	D1030	F1033	M1034	L1037	E1038	R1039	Y1040	K1047	L1048	M1049	R1053	A1054	L1055	K1058	Y1059	E1067	E1071	D1082	Y1083	F1084	T1085	F1088	L1091	L1092	I1093	G1094	V1095	Y1096	M1097	I1098	V1099	N1102	L1103	S1104	D1105	L1106	Q1107	I1108	L1109	R1110	E1111	S1115									

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 6.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.286 , 0.317 0.282 , 0.311	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)	0.41 , 529.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.47	0/3437	0.81	3/4629 (0.1%)
1	B	0.46	0/3437	0.81	3/4629 (0.1%)
1	C	0.46	0/3437	0.81	3/4629 (0.1%)
1	D	0.46	0/3437	0.81	3/4629 (0.1%)
1	E	0.46	0/3437	0.81	3/4629 (0.1%)
1	F	0.46	0/3437	0.81	3/4629 (0.1%)
1	G	0.46	0/3437	0.81	3/4629 (0.1%)
All	All	0.46	0/24059	0.81	21/32403 (0.1%)

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.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	672	ASN	N-CA-C	-9.98	100.42	112.59
1	F	672	ASN	N-CA-C	-9.97	100.42	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	672	ASN	N-CA-C	-9.97	100.43	112.59
1	G	672	ASN	N-CA-C	-9.97	100.43	112.59
1	E	672	ASN	N-CA-C	-9.96	100.43	112.59
1	D	672	ASN	N-CA-C	-9.94	100.47	112.59
1	B	672	ASN	N-CA-C	-9.94	100.47	112.59
1	G	671	LYS	N-CA-C	8.45	121.32	109.15
1	A	671	LYS	N-CA-C	8.45	121.32	109.15
1	C	671	LYS	N-CA-C	8.45	121.31	109.15
1	D	671	LYS	N-CA-C	8.43	121.29	109.15
1	B	671	LYS	N-CA-C	8.43	121.28	109.15
1	E	671	LYS	N-CA-C	8.42	121.28	109.15
1	F	671	LYS	N-CA-C	8.40	121.25	109.15
1	D	695	GLN	N-CA-C	-5.98	106.23	112.93
1	E	695	GLN	N-CA-C	-5.98	106.23	112.93
1	C	695	GLN	N-CA-C	-5.97	106.24	112.93
1	F	695	GLN	N-CA-C	-5.96	106.25	112.93
1	G	695	GLN	N-CA-C	-5.93	106.29	112.93
1	B	695	GLN	N-CA-C	-5.93	106.29	112.93
1	A	695	GLN	N-CA-C	-5.92	106.29	112.93

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 ⓘ

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	132	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3399	0	3409	132	0
1	C	3399	0	3409	132	1
1	D	3399	0	3409	139	0
1	E	3399	0	3409	137	7
1	F	3399	0	3409	132	0
1	G	3399	0	3409	133	0
All	All	23793	0	23863	913	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 19.

All (913) 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
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:1034:MET:HE2	1:B:1034:MET:HA	1.67	0.77
1:F:1034:MET:HE2	1:F:1034:MET:HA	1.67	0.77
1:C:1034:MET:HA	1:C:1034:MET:HE2	1.67	0.77
1:G:1034:MET:HE2	1:G:1034:MET:HA	1.67	0.77
1:E:1034:MET:HA	1:E:1034:MET:HE2	1.67	0.77
1:D:1034:MET:HE2	1:D:1034:MET:HA	1.67	0.76
1:B:761:VAL:HG11	1:C:840:SEP:O2P	1.86	0.76
1:A:1034:MET:HE2	1:A:1034:MET:HA	1.67	0.75
1:F:1108:ILE:CD1	1:G:1059:TYR:OH	2.35	0.74
1:A:781:ILE:HG22	1:A:906:MET:HE2	1.69	0.74
1:D:781:ILE:HG22	1:D:906:MET:HE2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:781:ILE:HG22	1:B:906:MET:HE2	1.70	0.73
1:C:781:ILE:HG22	1:C:906:MET:HE2	1.70	0.73
1:F:781:ILE:HG22	1:F:906:MET:HE2	1.69	0.73
1:E:781:ILE:HG22	1:E:906:MET:HE2	1.70	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: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: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:D:715:GLU:HG3	1:D:829:PHE:HB2	1.71	0.71
1:G:781:ILE:HG22	1:G:906:MET:HE2	1.70	0.71
1:B:1010:MET:HE2	1:B:1010:MET:HA	1.73	0.70
1:C:730:ARG:HB3	1:C:746:GLU:HG2	1.74	0.70
1:E:910:PHE:CD2	1:E:960:MET:HE1	2.27	0.70
1:G:910:PHE:CD2	1:G:960:MET:HE1	2.27	0.70
1:A:1010:MET:HA	1:A:1010:MET:HE2	1.73	0.70
1:B:910:PHE:CD2	1:B:960:MET:HE1	2.27	0.70
1:E:1010:MET:HE2	1:E:1010:MET:HA	1.73	0.70
1:G:1010:MET:HE2	1:G:1010:MET:HA	1.73	0.70
1:D:848:ASN:HB3	1:D:849:PRO:CA	2.21	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: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:D:1010:MET:HE2	1:D:1010:MET:HA	1.73	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:C:725:HIS:CD2	1:C:727:ASN:H	2.10	0.69
1:C:1010:MET:HE2	1:C:1010:MET:HA	1.73	0.69
1:E:862:GLU:HG3	1:E:863:GLU:N	2.07	0.69
1:G:848:ASN:HB3	1:G:849:PRO:CA	2.21	0.69
1:A:910:PHE:CD2	1:A:960:MET:HE1	2.27	0.69
1:B:862:GLU:HG3	1:B:863:GLU:N	2.07	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:C:910:PHE:CD2	1:C:960:MET:HE1	2.27	0.69
1:D:910:PHE:CD2	1:D:960:MET:HE1	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:1010:MET:HA	1:F:1010:MET:HE2	1.73	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:F:910:PHE:CD2	1:F:960:MET:HE1	2.27	0.68
1:A:795:HIS:HA	1:A:832:CYS:HB3	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: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:864:SER:HB3	1:B:963:HIS:NE2	2.12	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
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:B:1034:MET:CE	1:B:1037:LEU:HD23	2.28	0.64
1:G:1034:MET:CE	1:G:1037:LEU:HD23	2.28	0.64
1:F:864:SER:HB3	1:F:963:HIS:NE2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:864:SER:HB3	1:A:963:HIS:NE2	2.12	0.63
1:C:1034:MET:CE	1:C:1037:LEU:HD23	2.28	0.63
1:F:1108:ILE:HD11	1:G:1059:TYR:OH	1.96	0.63
1:A:1034:MET:HE1	1:A:1037:LEU:HD23	1.81	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: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:C:1034:MET:HE1	1:C:1037:LEU:HD23	1.81	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:D:1034:MET:HE1	1:D:1037:LEU:HD23	1.81	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:G:1034:MET:HE1	1:G:1037:LEU:HD23	1.81	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:1034:MET:HE1	1:E:1037:LEU:HD23	1.81	0.62
1:E:923:ASP:O	1:E:927:ARG:HB2	1.99	0.62
1:B:1034:MET:HE1	1:B:1037:LEU:HD23	1.81	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: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:F:1034:MET:HE1	1:F:1037:LEU:HD23	1.81	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
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:E:956:LEU:HG	1:E:960:MET:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:956:LEU:HG	1:F:960:MET:HE2	1.83	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:B:956:LEU:HG	1:B:960:MET:HE2	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:956:LEU:HG	1:C:960:MET:HE2	1.83	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:G:956:LEU:HG	1:G:960:MET:HE2	1.83	0.60
1:A:956:LEU:HG	1:A:960:MET:HE2	1.83	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:G:1055:LEU:HD23	1:G:1055:LEU:C	2.29	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:1055:LEU:C	1:B:1055:LEU:HD23	2.29	0.58
1:D:1055:LEU:C	1:D:1055:LEU:HD23	2.29	0.58
1:E:1055:LEU:HD23	1:E:1055:LEU:C	2.29	0.58
1:D:956:LEU:HG	1:D:960:MET:HE2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:761:VAL:HG21	1:A:764:GLU:HG3	1.85	0.58
1:C:1055:LEU:C	1:C:1055:LEU:HD23	2.29	0.58
1:A:861:LEU:O	1:A:862:GLU:HB3	2.04	0.57
1:B:782:ALA:HA	1:B:906:MET:HE1	1.86	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:D:782:ALA:HA	1:D:906:MET:HE1	1.86	0.57
1:A:1055:LEU:C	1:A:1055:LEU:HD23	2.29	0.57
1:B:761:VAL:HG21	1:B:764:GLU:HG3	1.85	0.57
1:A:782:ALA:HA	1:A:906:MET:HE1	1.86	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:F:1055:LEU:C	1:F:1055:LEU:HD23	2.29	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:F:782:ALA:HA	1:F:906:MET:HE1	1.86	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:G:782:ALA:HA	1:G:906:MET:HE1	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:861:LEU:O	1:F:862:GLU:HB3	2.04	0.55
1:C:782:ALA:HA	1:C:906:MET:HE1	1.86	0.55
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:E:782:ALA:HA	1:E:906:MET:HE1	1.86	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:A:785:VAL:HG21	1:A:906:MET:HE3	1.89	0.55
1:B:757:GLU:O	1:B:759:LYS:HE3	2.07	0.55
1:D:1047:LYS:HD3	1:D:1049:MET:HE3	1.89	0.55
1:E:785:VAL:HG21	1:E:906:MET:HE3	1.89	0.55
1:C:749:ASN:OD1	1:C:749:ASN:N	2.39	0.55
1:G:785:VAL:HG21	1:G:906:MET:HE3	1.89	0.55
1:E:1047:LYS:HD3	1:E:1049:MET:HE3	1.89	0.54
1:G:1016:SER:C	1:G:1018:PHE:H	2.15	0.54
1:B:1016:SER:C	1:B:1018:PHE:H	2.15	0.54
1:C:1047:LYS:HD3	1:C:1049:MET:HE3	1.89	0.54
1:E:757:GLU:O	1:E:759:LYS:HE3	2.07	0.54
1:F:785:VAL:HG21	1:F:906:MET:HE3	1.89	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
1:A:752:LEU:HD21	1:A:913:ILE:HD11	1.90	0.54
1:B:673:LEU:HD23	1:B:673:LEU:C	2.33	0.54
1:C:737:THR:HG23	1:C:740:PHE:H	1.73	0.54
1:C:1016:SER:C	1:C:1018:PHE:H	2.15	0.54
1:D:673:LEU:C	1:D:673:LEU:HD23	2.33	0.54
1:E:673:LEU:HD23	1:E:673:LEU:C	2.33	0.54
1:E:824:ILE:O	1:E:825:LEU:HD23	2.08	0.54
1:F:673:LEU:C	1:F:673:LEU:HD23	2.33	0.54
1:A:757:GLU:O	1:A:759:LYS:HE3	2.07	0.54
1:A:1016:SER:C	1:A:1018:PHE:H	2.15	0.54
1:C:785:VAL:HG21	1:C:906:MET:HE3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:824:ILE:O	1:A:825:LEU:HD23	2.08	0.54
1:D:671:LYS:HD2	1:D:671:LYS:O	2.08	0.54
1:A:1047:LYS:HD3	1:A:1049:MET:HE3	1.89	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:1016:SER:C	1:D:1018:PHE:H	2.15	0.54
1:G:673:LEU:HD23	1:G:673:LEU:C	2.33	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:B:1047:LYS:HD3	1:B:1049:MET:HE3	1.89	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:1047:LYS:HD3	1:F:1049:MET:HE3	1.89	0.53
1:F:1111:GLU:O	1:F:1115:SER:HB3	2.09	0.53
1:G:1047:LYS:HD3	1:G:1049:MET:HE3	1.89	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:785:VAL:HG21	1:B:906:MET:HE3	1.89	0.53
1:B:1111:GLU:O	1:B:1115:SER:HB3	2.09	0.53
1:C:673:LEU:C	1:C:673:LEU:HD23	2.33	0.53
1:C:1111:GLU:O	1:C:1115:SER:HB3	2.09	0.53
1:D:785:VAL:HG21	1:D:906:MET:HE3	1.89	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:E:1016:SER:C	1:E:1018:PHE:H	2.15	0.53
1:A:673:LEU:C	1:A:673:LEU:HD23	2.33	0.53
1:E:723:ASP:HB2	1:E:730:ARG:HA	1.91	0.53
1:F:671:LYS:HD2	1:F:671:LYS:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:671:LYS:HD2	1:B:671:LYS:O	2.08	0.53
1:F:1016:SER:C	1:F:1018:PHE:H	2.15	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: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:F:928:GLU:O	1:F:932:ILE:HG13	2.10	0.52
1:F:1005:PRO:HB2	1:F:1010:MET:HE3	1.92	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:D:1005:PRO:HB2	1:D:1010:MET:HE3	1.92	0.52
1:F:1033:PHE:CE2	1:F:1034:MET:HE3	2.45	0.52
1:G:1005:PRO:HB2	1:G:1010:MET:HE3	1.92	0.52
1:B:749:ASN:OD1	1:B:749:ASN:N	2.39	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:E:1033:PHE:CE2	1:E:1034:MET:HE3	2.45	0.52
1:A:1033:PHE:CE2	1:A:1034:MET:HE3	2.45	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:C:1033:PHE:CE2	1:C:1034:MET:HE3	2.45	0.52
1:D:737:THR:HG23	1:D:740:PHE:H	1.73	0.52
1:D:1033:PHE:CE2	1:D:1034:MET:HE3	2.45	0.52
1:F:941:MET:HE3	1:F:950:ILE:HG23	1.91	0.52
1:G:729:ILE:CD1	1:G:745:LEU:HB3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1033:PHE:CE2	1:G:1034:MET:HE3	2.45	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
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:C:941:MET:HE3	1:C:950:ILE:HG23	1.91	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:C:1037:LEU:C	1:C:1039:ARG:H	2.18	0.51
1:B:928:GLU:O	1:B:932:ILE:HG13	2.10	0.51
1:B:941:MET:HE3	1:B:950:ILE:HG23	1.91	0.51
1:A:737:THR:C	1:A:739:ARG:H	2.19	0.51
1:B:737:THR:C	1:B:739:ARG:H	2.19	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:B:1037:LEU:C	1:B:1039:ARG:H	2.18	0.51
1:C:1005:PRO:HB2	1:C:1010:MET:HE3	1.92	0.51
1:D:1037:LEU:C	1:D:1039:ARG:H	2.18	0.51
1:E:731:TYR:HA	1:E:745:LEU:HD23	1.92	0.51
1:F:737:THR:C	1:F:739:ARG:H	2.19	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:D:941:MET:HE3	1:D:950:ILE:HG23	1.91	0.51
1:E:737:THR:C	1:E:739:ARG:H	2.19	0.51
1:G:941:MET:HE3	1:G:950:ILE:HG23	1.91	0.51
1:A:941:MET:HE3	1:A:950:ILE:HG23	1.91	0.51
1:A:1005:PRO:HB2	1:A:1010:MET:HE3	1.92	0.51
1:D:737:THR:C	1:D:739:ARG:H	2.19	0.51
1:E:811:PHE:HB3	1:E:823:ARG:NH1	2.26	0.51
1:G:737:THR:C	1:G:739:ARG:H	2.19	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:E:941:MET:HE3	1:E:950:ILE:HG23	1.91	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:B:1005:PRO:HB2	1:B:1010:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1033:PHE:CE2	1:B:1034:MET:HE3	2.45	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:A:1037:LEU:C	1:A:1039:ARG:H	2.18	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:G:1037:LEU:C	1:G:1039:ARG:H	2.18	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:C:737:THR:C	1:C:739:ARG:H	2.19	0.50
1:F:758:SER:HB3	1:F:768:LEU:HD21	1.93	0.50
1:F:845:ASN:N	1:F:845:ASN:HD22	2.08	0.50
1:E:1005:PRO:HB2	1:E:1010:MET:HE3	1.92	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
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:1037:LEU:C	1:F:1039:ARG:H	2.18	0.50
1:G:758:SER:HB3	1:G:768:LEU:HD21	1.93	0.50
1:E:845:ASN:N	1:E:845:ASN:HD22	2.08	0.50
1:E:1037:LEU:C	1:E:1039:ARG:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:731:TYR:HA	1:G:745:LEU:HD23	1.92	0.49
1:D:845:ASN:N	1:D:845:ASN:HD22	2.08	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
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: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: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:C:1000:GLU:HB2	1:C:1009:LEU:HD21	1.93	0.49
1:A:781:ILE:HG22	1:A:906:MET:CE	2.41	0.49
1:B:924:LYS:HG3	1:B:925:TYR:CD2	2.47	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: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:C:1103:LEU:C	1:C:1105:ASP:H	2.22	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:D:970:THR:HG23	1:D:973:LYS:CB	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:1034:MET:HA	1:G:1034:MET:CE	2.42	0.48
1:G:1103:LEU:C	1:G:1105:ASP:H	2.22	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:E:1103:LEU:C	1:E:1105:ASP:H	2.22	0.48
1:A:1103:LEU:C	1:A:1105:ASP:H	2.22	0.48
1:G:893:THR:O	1:G:895:ARG:HG3	2.14	0.48
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: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:E:1020:ILE:HG22	1:E:1021:PRO:C	2.39	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:B:1020:ILE:HG22	1:B:1021:PRO:C	2.39	0.47
1:E:970:THR:HG23	1:E:973:LYS:CB	2.43	0.47
1:B:1103:LEU:C	1:B:1105:ASP:H	2.22	0.47
1:C:674:VAL:CG1	1:C:675:VAL:N	2.76	0.47
1:C:1020:ILE:HG22	1:C:1021:PRO:C	2.39	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: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:F:1020:ILE:HG22	1:F:1021:PRO:C	2.39	0.47
1:G:781:ILE:HG22	1:G:906:MET:CE	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1103:LEU:C	1:D:1105:ASP:H	2.22	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:F:1103:LEU:C	1:F:1105:ASP:H	2.22	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: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
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: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:G:1020:ILE:HG22	1:G:1021:PRO:C	2.39	0.47
1:A:1034:MET:HA	1:A:1034:MET:CE	2.42	0.46
1:C:970:THR:HG23	1:C:973:LYS:CB	2.44	0.46
1:D:1020:ILE:HG22	1:D:1021:PRO:C	2.39	0.46
1:A:725:HIS:CG	1:A:726:PRO:HD2	2.50	0.46
1:A:837:SER:CB	1:A:838:GLY:HA2	2.45	0.46
1:C:804:LEU:HB2	1:C:825:LEU:HB2	1.97	0.46
1:A:804:LEU:HB2	1:A:825:LEU:HB2	1.97	0.46
1:A:1020:ILE:HG22	1:A:1021:PRO:C	2.39	0.46
1:B:687:THR:HG23	1:B:704:MET:HG2	1.98	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: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: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:F:1048:LEU:O	1:F:1049:MET:C	2.59	0.46
1:A:794:ILE:O	1:A:832:CYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1048:LEU:O	1:A:1049:MET:C	2.59	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:F:672:ASN:H	1:F:672:ASN:ND2	2.13	0.46
1:G:794:ILE:O	1:G:832:CYS:HB2	2.16	0.46
1:G:837:SER:CB	1:G:838:GLY:HA2	2.45	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:D:914:LEU:O	1:D:943:CYS:HB2	2.16	0.46
1:D:1033:PHE:CD2	1:D:1034:MET:HE3	2.51	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:E:1034:MET:HA	1:E:1034:MET:CE	2.42	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:C:1048:LEU:O	1:C:1049:MET:C	2.59	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:1033:PHE:CD2	1:F:1034:MET:HE3	2.51	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:D:864:SER:O	1:D:893:THR:OG1	2.29	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:D:1048:LEU:O	1:D:1049:MET:C	2.59	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:E:1048:LEU:O	1:E:1049:MET:C	2.59	0.45
1:F:794:ILE:N	1:F:794:ILE:HD12	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:964:ASP:HA	1:F:965:PRO:HD2	1.84	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:B:1033:PHE:CD2	1:B:1034:MET:HE3	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: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:857:ALA:O	1:G:860:LEU:HB2	2.16	0.45
1:B:1034:MET:HA	1:B:1034:MET:CE	2.42	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: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:B:1048:LEU:O	1:B:1049:MET:C	2.59	0.45
1:E:685:SER:HB3	1:E:708:PHE:CZ	2.51	0.45
1:A:1033:PHE:CD2	1:A:1034:MET:HE3	2.51	0.45
1:C:1033:PHE:CD2	1:C:1034:MET:HE3	2.51	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:781:ILE:HG22	1:C:906:MET:CE	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:864:SER:O	1:F:893:THR:OG1	2.29	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
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:G:1048:LEU:O	1:G:1049:MET:C	2.59	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:781:ILE:HG22	1:F:906:MET:CE	2.41	0.44
1:F:946:ASP:HB3	1:F:949:LEU:HD12	1.99	0.44
1:G:1033:PHE:CD2	1:G:1034:MET:HE3	2.51	0.44
1:G:1082:ASP:HA	1:G:1085:THR:HB	1.99	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:E:1033:PHE:CD2	1:E:1034:MET:HE3	2.51	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:895:ARG:HH12	1:A:964:ASP:CG	2.26	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:G:895:ARG:HH12	1:G:964:ASP:CG	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:719:LEU:HD23	1:C:719:LEU:HA	1.71	0.43
1:C:895:ARG:HH12	1:C:964:ASP:CG	2.26	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: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
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:D:895:ARG:HH12	1:D:964:ASP:CG	2.26	0.43
1:B:791:LEU:C	1:B:792:LYS:HD3	2.44	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:791:LEU:C	1:G:792:LYS:HD3	2.44	0.43
1:G:925:TYR:CD2	1:G:925:TYR:N	2.87	0.43
1:A:791:LEU:C	1:A:792:LYS:HD3	2.44	0.43
1:A:906:MET:HE3	1:A:906:MET:HB2	1.88	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:791:LEU:C	1:F:792:LYS:HD3	2.44	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:E:758:SER:CB	1:E:768:LEU:HD21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:845:ASN:N	1:E:845:ASN:ND2	2.66	0.43
1:E:895:ARG:HH12	1:E:964:ASP:CG	2.26	0.43
1:F:758:SER:CB	1:F:768:LEU:HD21	2.49	0.43
1:F:1034:MET:HA	1:F:1034:MET:CE	2.42	0.43
1:A:758:SER:CB	1:A:768:LEU:HD21	2.49	0.43
1:B:845:ASN:C	1:B:846:LEU:HD22	2.44	0.43
1:C:729:ILE:HD12	1:C:745:LEU:HB3	2.01	0.43
1:D:791:LEU:C	1:D:792:LYS:HD3	2.44	0.43
1:F:845:ASN:C	1:F:846:LEU:HD22	2.44	0.43
1:B:1008:LEU:HD23	1:B:1008:LEU:HA	1.76	0.43
1:D:845:ASN:N	1:D:845:ASN:ND2	2.66	0.43
1:D:845:ASN:C	1:D:846:LEU:HD22	2.44	0.43
1:E:845:ASN:C	1:E:846:LEU:HD22	2.44	0.43
1:A:845:ASN:N	1:A:845:ASN:ND2	2.66	0.42
1:C:791:LEU:C	1:C:792:LYS:HD3	2.44	0.42
1:G:758:SER:CB	1:G:768:LEU:HD21	2.49	0.42
1:D:1034:MET:HA	1:D:1034:MET:CE	2.42	0.42
1:F:729:ILE:HD12	1:F:745:LEU:HB3	2.01	0.42
1:D:999:ILE:N	1:D:999:ILE:HD12	2.34	0.42
1:F:798:LEU:HD23	1:F:798:LEU:HA	1.80	0.42
1:F:895:ARG:HH12	1:F:964:ASP:CG	2.26	0.42
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: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: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:A:845:ASN:C	1:A:846:LEU:HD22	2.44	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:B:895:ARG:HH12	1:B:964:ASP:CG	2.26	0.42
1:C:898:THR:HG23	1:C:900:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:799:LYS:NZ	1:C:852:THR:HG23	2.35	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: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:E:799:LYS:NZ	1:E:852:THR:HG23	2.35	0.42
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:C:845:ASN:C	1:C:846:LEU:HD22	2.44	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:E:791:LEU:C	1:E:792:LYS:HD3	2.44	0.42
1:E:864:SER:O	1:E:893:THR:OG1	2.29	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:C:1008:LEU:HD23	1:C:1008:LEU:HA	1.77	0.41
1:D:1030:ASP:OD1	1:D:1030:ASP:N	2.53	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:C:1034:MET:HA	1:C:1034:MET:CE	2.42	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:845:ASN:C	1:G:846:LEU:HD22	2.44	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:787:HIS:O	1:E:790:SER:HB2	2.20	0.41
1:E:906:MET:HE3	1:E:906:MET:HB2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:694:PHE:C	1:A:696:GLY:H	2.29	0.41
1:A:725:HIS:CD2	1:A:727:ASN:HB2	2.55	0.41
1:A:797:ASP:O	1:A:798:LEU:C	2.64	0.41
1:B:906:MET:HE3	1:B:906:MET:HB2	1.88	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:B:792:LYS:HE2	1:B:792:LYS:HB2	1.88	0.41
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:G:694:PHE:CG	1:G:695:GLN:N	2.87	0.41
1:E:848:ASN:CB	1:E:849:PRO:HA	2.29	0.41
1:F:797:ASP:O	1:F:798:LEU:C	2.64	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: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:797:ASP:O	1:C:798:LEU:C	2.64	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:E:811:PHE:HB3	1:E:823:ARG:HG3	2.03	0.41
1:F:899:ARG:C	1:F:901:ILE:N	2.79	0.41
1:G:712:ALA:O	1:G:716:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:797:ASP:O	1:B:798:LEU:C	2.64	0.41
1:B:1030:ASP:OD1	1:B:1030:ASP:N	2.53	0.41
1:C:798:LEU:HD23	1:C:798:LEU:HA	1.80	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:B:926:SER:O	1:B:927:ARG:C	2.65	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:D:694:PHE:C	1:D:696:GLY:H	2.29	0.40
1:E:785:VAL:HG21	1:E:906:MET:CE	2.52	0.40
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:G:899:ARG:C	1:G:901:ILE:N	2.79	0.40
1:G:1037:LEU:C	1:G:1039:ARG:N	2.80	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:899:ARG:C	1:C:901:ILE:N	2.79	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:ARG:C	1:B:901:ILE:N	2.79	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:E:708:PHE:O	1:E:709:CYS:C	2.65	0.40
1:E:797:ASP:O	1:E:798:LEU:C	2.64	0.40
1:E:1037:LEU:C	1:E:1039:ARG:N	2.80	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:694:PHE:C	1:B:696:GLY:H	2.29	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:1030:ASP:OD1	1:A:1030:ASP:N	2.53	0.40
1:A:1055:LEU:HD23	1:A:1055:LEU:O	2.21	0.40
1:C:694:PHE:C	1:C:696:GLY:H	2.29	0.40
1:C:1055:LEU:HD23	1:C:1055:LEU:O	2.21	0.40
1:E:694:PHE:C	1:E:696:GLY:H	2.29	0.40
1:E:926:SER:O	1:E:927:ARG:C	2.65	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
1:G:708:PHE:O	1:G:709:CYS:C	2.65	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	B	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	C	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	D	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	E	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	F	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	G	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
All	All	2891/3136 (92%)	2464 (85%)	364 (13%)	63 (2%)	5	29

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	E	849	PRO
1	F	849	PRO
1	G	849	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	B	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	C	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	D	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	E	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	F	380/405 (94%)	348 (92%)	32 (8%)	10	30
1	G	380/405 (94%)	348 (92%)	32 (8%)	10	30
All	All	2660/2835 (94%)	2436 (92%)	224 (8%)	10	30

All (224) 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
1	A	674	VAL
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	775	ILE
1	A	788	LEU
1	A	796	ARG

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Mol	Chain	Res	Type
1	A	804	LEU
1	A	817	THR
1	A	823	ARG
1	A	835	LEU
1	A	845	ASN
1	A	897	LEU
1	A	906	MET
1	A	939	ASP
1	A	943	CYS
1	A	970	THR
1	A	987	LEU
1	A	1020	ILE
1	A	1030	ASP
1	A	1048	LEU
1	A	1053	ARG
1	A	1067	GLU
1	A	1085	THR
1	A	1102	ASN
1	B	670	LEU
1	B	671	LYS
1	B	672	ASN
1	B	674	VAL
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	775	ILE
1	B	788	LEU
1	B	796	ARG
1	B	804	LEU
1	B	817	THR
1	B	823	ARG
1	B	835	LEU
1	B	845	ASN
1	B	897	LEU
1	B	906	MET
1	B	939	ASP
1	B	943	CYS
1	B	970	THR

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Mol	Chain	Res	Type
1	B	987	LEU
1	B	1020	ILE
1	B	1030	ASP
1	B	1048	LEU
1	B	1053	ARG
1	B	1067	GLU
1	B	1085	THR
1	B	1102	ASN
1	C	670	LEU
1	C	671	LYS
1	C	672	ASN
1	C	674	VAL
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	775	ILE
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	845	ASN
1	C	897	LEU
1	C	906	MET
1	C	939	ASP
1	C	943	CYS
1	C	970	THR
1	C	987	LEU
1	C	1020	ILE
1	C	1030	ASP
1	C	1048	LEU
1	C	1053	ARG
1	C	1067	GLU
1	C	1085	THR
1	C	1102	ASN
1	D	670	LEU
1	D	671	LYS

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Mol	Chain	Res	Type
1	D	672	ASN
1	D	674	VAL
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	775	ILE
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	845	ASN
1	D	897	LEU
1	D	906	MET
1	D	939	ASP
1	D	943	CYS
1	D	970	THR
1	D	987	LEU
1	D	1020	ILE
1	D	1030	ASP
1	D	1048	LEU
1	D	1053	ARG
1	D	1067	GLU
1	D	1085	THR
1	D	1102	ASN
1	E	670	LEU
1	E	671	LYS
1	E	672	ASN
1	E	674	VAL
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	775	ILE

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Mol	Chain	Res	Type
1	E	788	LEU
1	E	796	ARG
1	E	804	LEU
1	E	817	THR
1	E	823	ARG
1	E	835	LEU
1	E	845	ASN
1	E	897	LEU
1	E	906	MET
1	E	939	ASP
1	E	943	CYS
1	E	970	THR
1	E	987	LEU
1	E	1020	ILE
1	E	1030	ASP
1	E	1048	LEU
1	E	1053	ARG
1	E	1067	GLU
1	E	1085	THR
1	E	1102	ASN
1	F	670	LEU
1	F	671	LYS
1	F	672	ASN
1	F	674	VAL
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	775	ILE
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	845	ASN
1	F	897	LEU
1	F	906	MET
1	F	939	ASP

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Mol	Chain	Res	Type
1	F	943	CYS
1	F	970	THR
1	F	987	LEU
1	F	1020	ILE
1	F	1030	ASP
1	F	1048	LEU
1	F	1053	ARG
1	F	1067	GLU
1	F	1085	THR
1	F	1102	ASN
1	G	670	LEU
1	G	671	LYS
1	G	672	ASN
1	G	674	VAL
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	775	ILE
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	845	ASN
1	G	897	LEU
1	G	906	MET
1	G	939	ASP
1	G	943	CYS
1	G	970	THR
1	G	987	LEU
1	G	1020	ILE
1	G	1030	ASP
1	G	1048	LEU
1	G	1053	ARG
1	G	1067	GLU
1	G	1085	THR
1	G	1102	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) 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	773	ASN
1	A	839	GLN
1	A	845	ASN
1	A	1001	ASN
1	A	1061	HIS
1	A	1090	ASN
1	A	1102	ASN
1	B	672	ASN
1	B	691	GLN
1	B	725	HIS
1	B	753	GLN
1	B	773	ASN
1	B	839	GLN
1	B	845	ASN
1	B	1001	ASN
1	B	1061	HIS
1	B	1090	ASN
1	C	672	ASN
1	C	691	GLN
1	C	725	HIS
1	C	753	GLN
1	C	773	ASN
1	C	845	ASN
1	C	1001	ASN
1	C	1061	HIS
1	C	1090	ASN
1	C	1102	ASN
1	D	672	ASN
1	D	725	HIS
1	D	753	GLN
1	D	773	ASN
1	D	845	ASN
1	D	1001	ASN
1	D	1061	HIS
1	D	1090	ASN
1	E	672	ASN
1	E	691	GLN

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Mol	Chain	Res	Type
1	E	725	HIS
1	E	753	GLN
1	E	773	ASN
1	E	839	GLN
1	E	845	ASN
1	E	1001	ASN
1	E	1061	HIS
1	E	1090	ASN
1	E	1102	ASN
1	F	672	ASN
1	F	691	GLN
1	F	725	HIS
1	F	753	GLN
1	F	773	ASN
1	F	839	GLN
1	F	845	ASN
1	F	1001	ASN
1	F	1061	HIS
1	F	1090	ASN
1	G	672	ASN
1	G	691	GLN
1	G	725	HIS
1	G	753	GLN
1	G	773	ASN
1	G	839	GLN
1	G	845	ASN
1	G	1001	ASN
1	G	1061	HIS
1	G	1090	ASN
1	G	1102	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	F	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	SEP	C	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.40	1 (14%)
1	SEP	D	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.41	1 (14%)
1	SEP	A	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	TPO	E	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	SEP	F	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.41	1 (14%)
1	TPO	C	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	SEP	A	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.42	1 (14%)
1	TPO	G	844	1	8,10,11	3.11	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	C	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.74	0
1	SEP	G	841	1	8,9,10	1.58	1 (12%)	7,12,14	0.74	0
1	TPO	D	844	1	8,10,11	3.10	5 (62%)	10,14,16	1.65	2 (20%)
1	SEP	D	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	SEP	G	840	1	8,9,10	1.65	1 (12%)	7,12,14	1.39	1 (14%)
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	B	841	1	8,9,10	1.58	1 (12%)	7,12,14	0.74	0
1	TPO	A	844	1	8,10,11	3.10	5 (62%)	10,14,16	1.64	2 (20%)
1	TPO	B	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	TPO	F	844	1	8,10,11	3.12	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	F	841	1	-	1/6/8/10	-
1	SEP	C	840	1	-	4/6/8/10	-
1	SEP	D	840	1	-	4/6/8/10	-
1	SEP	A	841	1	-	1/6/8/10	-

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.15	36 (8%) 16 23	53, 108, 202, 287	0
1	B	415/448 (92%)	-0.04	20 (4%) 35 37	53, 108, 202, 287	0
1	C	415/448 (92%)	-0.41	3 (0%) 84 74	53, 108, 202, 287	0
1	D	415/448 (92%)	-0.31	5 (1%) 76 65	53, 108, 202, 287	0
1	E	415/448 (92%)	-0.24	8 (1%) 66 56	53, 108, 202, 287	0
1	F	415/448 (92%)	-0.16	10 (2%) 59 52	53, 108, 202, 287	0
1	G	415/448 (92%)	-0.15	12 (2%) 53 47	53, 108, 202, 287	0
All	All	2905/3136 (92%)	-0.17	94 (3%) 50 45	53, 108, 203, 287	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1058	LYS	8.9
1	B	860	LEU	7.5
1	A	1033	PHE	6.7
1	B	853	SER	5.9
1	B	856	ARG	5.5
1	G	860	LEU	5.3
1	A	864	SER	5.1
1	A	997	LEU	4.9
1	D	1033	PHE	4.8
1	F	1040	TYR	4.6
1	A	1084	PHE	4.5
1	A	861	LEU	4.5
1	G	1084	PHE	4.5
1	A	1036	ASN	4.2
1	B	861	LEU	4.2
1	E	897	LEU	4.1
1	E	746	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	998	GLU	4.0
1	B	801	GLN	4.0
1	G	1033	PHE	4.0
1	A	990	LEU	3.9
1	B	1091	LEU	3.8
1	A	1073	MET	3.7
1	A	859	GLU	3.7
1	A	1037	LEU	3.6
1	A	1055	LEU	3.3
1	A	1054	ALA	3.3
1	F	859	GLU	3.2
1	A	860	LEU	3.1
1	E	747	LEU	3.1
1	A	1091	LEU	3.1
1	B	1084	PHE	3.1
1	B	897	LEU	3.1
1	A	1072	LEU	3.0
1	F	1058	LYS	3.0
1	B	1033	PHE	3.0
1	A	1052	LEU	3.0
1	E	864	SER	3.0
1	A	995	ASP	2.9
1	A	858	PRO	2.9
1	A	862	GLU	2.9
1	A	1041	ARG	2.8
1	A	993	VAL	2.8
1	A	999	ILE	2.8
1	B	1052	LEU	2.8
1	A	1109	LEU	2.7
1	A	1080	PHE	2.7
1	G	1029	PHE	2.7
1	G	897	LEU	2.6
1	B	864	SER	2.6
1	B	1026	THR	2.6
1	C	860	LEU	2.6
1	A	1040	TYR	2.6
1	C	1058	LYS	2.6
1	A	1056	ARG	2.6
1	A	1064	ASP	2.5
1	G	1091	LEU	2.5
1	C	1033	PHE	2.5
1	D	1034	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	1037	LEU	2.4
1	B	932	ILE	2.4
1	F	1052	LEU	2.4
1	F	724	ASP	2.4
1	G	794	ILE	2.4
1	F	860	LEU	2.4
1	B	854	GLY	2.4
1	D	1012	PHE	2.4
1	G	1034	MET	2.4
1	D	1037	LEU	2.3
1	F	897	LEU	2.3
1	E	842	PHE	2.3
1	A	738	ASP	2.3
1	A	996	ARG	2.3
1	D	1084	PHE	2.3
1	F	1084	PHE	2.3
1	E	860	LEU	2.2
1	B	855	TRP	2.2
1	A	739	ARG	2.2
1	E	853	SER	2.2
1	A	1053	ARG	2.2
1	B	696	GLY	2.2
1	G	1040	TYR	2.2
1	B	1037	LEU	2.2
1	G	966	LEU	2.2
1	B	776	SER	2.2
1	B	709	CYS	2.2
1	F	760	ASN	2.1
1	F	1033	PHE	2.1
1	A	1059	TYR	2.1
1	A	853	SER	2.1
1	A	1051	LEU	2.1
1	E	1025	TRP	2.0
1	B	710	ASP	2.0
1	G	856	ARG	2.0

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

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($\text{\AA}^2$)	Q<0.9
1	SEP	E	841	10/11	0.48	0.18	111,133,156,162	0
1	TPO	A	844	11/12	0.49	0.12	166,194,212,216	0
1	TPO	C	844	11/12	0.52	0.09	166,194,212,216	0
1	TPO	G	844	11/12	0.57	0.07	166,194,212,216	0
1	SEP	C	841	10/11	0.63	0.13	111,133,156,162	0
1	TPO	B	844	11/12	0.65	0.07	166,194,212,216	0
1	TPO	E	844	11/12	0.69	0.06	166,194,212,216	0
1	SEP	G	841	10/11	0.73	0.06	111,133,156,162	0
1	SEP	A	841	10/11	0.76	0.09	111,133,156,162	0
1	TPO	D	844	11/12	0.76	0.07	166,194,212,216	0
1	SEP	E	840	10/11	0.77	0.18	147,153,162,164	0
1	SEP	B	840	10/11	0.81	0.09	147,153,162,164	0
1	SEP	A	840	10/11	0.81	0.08	147,153,162,164	0
1	SEP	D	841	10/11	0.83	0.07	111,133,156,162	0
1	SEP	C	840	10/11	0.84	0.13	147,153,162,164	0
1	SEP	D	840	10/11	0.85	0.06	147,153,162,164	0
1	SEP	F	840	10/11	0.85	0.10	147,153,162,164	0
1	SEP	B	841	10/11	0.86	0.10	111,133,156,162	0
1	SEP	G	840	10/11	0.86	0.11	147,153,162,164	0
1	SEP	F	841	10/11	0.88	0.06	111,133,156,162	0
1	TPO	F	844	11/12	0.89	0.04	166,194,212,216	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.