



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 AM GMT

PDB ID : 2X6J
Title : THE CRYSTAL STRUCTURE OF THE DROSOPHILA CLASS III PI3-KINASE VPS34 IN COMPLEX WITH PIK-93
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Deposited on : 2010-02-17
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

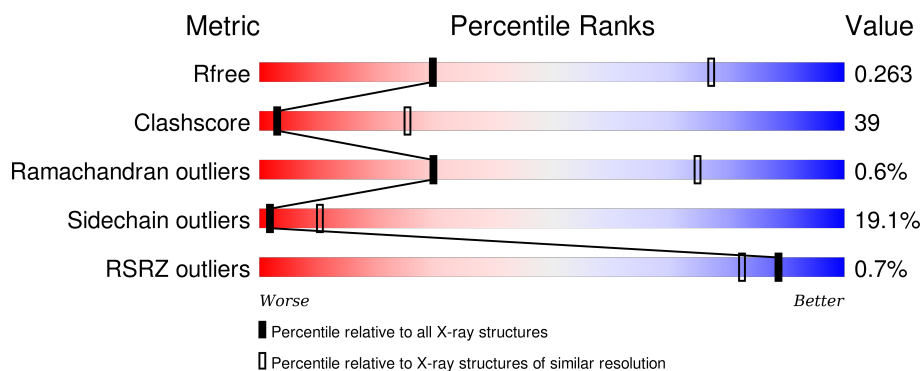
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	696	 34% 34% 10% 22%
1	B	696	 34% 34% 10% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8967 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.

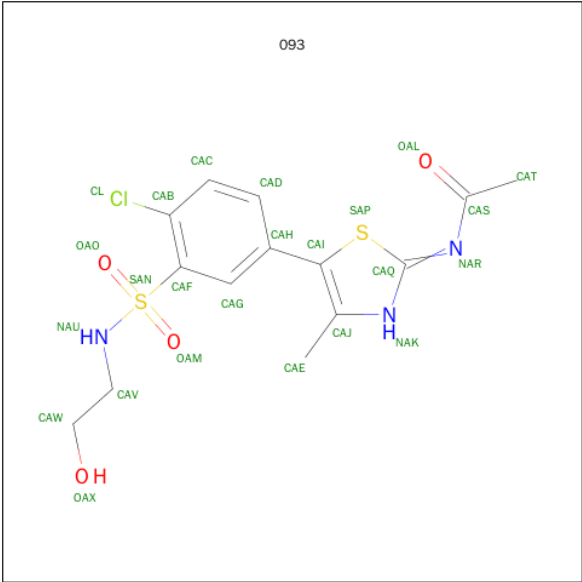
- Molecule 1 is a protein called PHOSPHOTIDYLINOSITOL 3 KINASE 59F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4457	2882	757	791	27			
1	B	546	Total	C	N	O	S	0	0	0
			4462	2886	759	790	27			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	EXPRESSION TAG	UNP Q9W1M7
A	255	SER	-	EXPRESSION TAG	UNP Q9W1M7
A	256	HIS	-	EXPRESSION TAG	UNP Q9W1M7
A	257	MET	-	EXPRESSION TAG	UNP Q9W1M7
A	455	ALA	GLY	ENGINEERED MUTATION	UNP Q9W1M7
B	254	GLY	-	EXPRESSION TAG	UNP Q9W1M7
B	255	SER	-	EXPRESSION TAG	UNP Q9W1M7
B	256	HIS	-	EXPRESSION TAG	UNP Q9W1M7
B	257	MET	-	EXPRESSION TAG	UNP Q9W1M7
B	455	ALA	GLY	ENGINEERED MUTATION	UNP Q9W1M7

- Molecule 2 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIAZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: C₁₄H₁₆ClN₃O₄S₂).

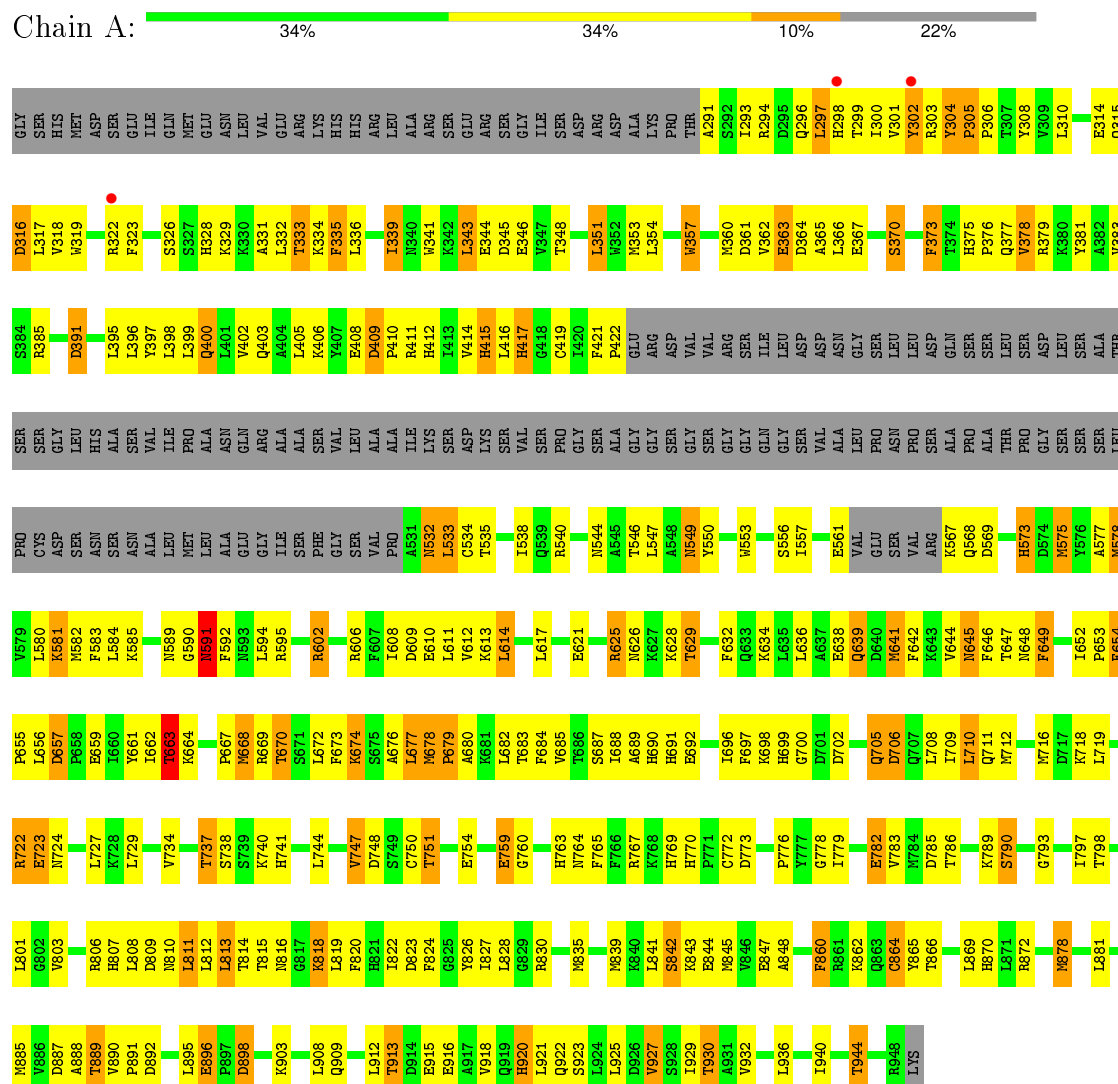


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			24	14	1	3	4	2		
2	B	1	Total	C	Cl	N	O	S	0	0
			24	14	1	3	4	2		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: PHOSPHOTIDYLINOSITOL 3 KINASE 59F



• Molecule 1: PHOSPHOTIDYLINOSITOL 3 KINASE 59F



F882	D805	Y732	P653	K581	LEU	THR	A382	E314	GLY
A888	R806	Y733	F654	M582	PRO	SER	A382	Q315	SER
T889	H807	A734	P655	V586	CYS	HIS	R385	D316	HIS
V890	L808	L656	V586	L587	ASP	GLY	Q388	L317	MET
P891	D809	L735	P657	L587	SER	LEU	Q388	V318	ASP
D892	N810	A736	Q590	Q590	ASN	HIS	Q388	W319	SER
L893	L811	T737	Y661	M591	SER	ALA	Q388	K320	GLU
A894	L812	S738	I662	M591	ASN	SER	D391	F321	ILE
L895	L813	S739	I662	L594	ALA	VAL	E392	R322	GLN
E896	T814	K740	T663	L594	LEU	ILE	D393	K322	MET
P897	T815	H741	K664	R595	MET	PRO	L325	L325	GLU
G817	N816	G742	P667	F598	LEU	ALA	L398	S326	ASN
P898	G817	F743	P667	Y599	ALA	ASN	L399	S327	LEU
K899	K818	L744	T670	M600	GLU	GLN	Q400	K328	VAL
K903	L819	V747	S671	R602	GLY	ARG	L401	K329	GLU
E906	F820	D748	L672	L601	ILE	ALA	V402	K330	ARG
I907	H821	S749	F673	K603	SER	ALA	L405	A331	LYS
D923	D823	G750	Q604	Q604	PHE	SER	L406	L332	HIS
F824	F824	T751	R605	R605	GLY	VAL	Y407	T333	HIS
E825	G825	A752	P679	P679	SER	LEU	E408	K334	ARG
Y826	Y826	A753	L677	L677	VAL	ALA	F335	F335	LEU
I827	I827	E754	M608	M608	PRO	ALA	D409	K336	ALA
L828	L828	V755	E610	E610	ALA	ILE	P410	K337	ARG
G829	G829	L756	T686	L611	LYS	SER	H412	C338	SER
R830	R830	A757	H691	L614	ASP	ASP	I413	I339	GLU
M835	M835	R758	I696	V618	LYS	LYS	H414	K340	ARG
P836	P836	E759	F697	V618	GLY	GLY	K342	K341	SER
P837	P837	H763	K698	E621	VAL	VAL	L343	K342	ILE
P838	P838	I764	K698	E621	SER	SER	E344	L343	ILE
M839	M839	F765	H699	E622	PRO	PRO	D345	D345	ASP
K840	K840	F766	G700	G623	GLY	GLY	E346	E346	ARG
L841	L841	R767	D702	M624	SER	SER	V347	V347	ASP
S842	S842	F771	D702	R625	ALA	ALA	T348	T348	LYS
K843	K843	G772	L703	M626	GLY	GLY	E423	Q349	LYS
A848	A848	D773	R704	K627	ASP	ASP	ASP	PRO	THR
P849	P849	D773	Q705	K628	SER	SER	VAL	THR	THR
G850	G850	F776	D706	K628	GLY	GLY	VAL	L354	L291
G851	G851	Y777	Q707	E630	GLY	GLY	ARG	S292	S292
I852	I852	G778	L708	E630	GLY	GLY	ARG	L293	L293
S853	S853	I779	L709	F631	ILE	ILE	SER	K294	K294
S854	S854	I779	L710	Q633	GLY	GLY	ILE	D295	D295
E855	E855	H712	Q711	K634	VAL	VAL	LEU	Q296	Q296
E859	E859	E782	H712	L635	SER	SER	ASP	L297	L297
F860	F860	V783	I713	L636	GLU	GLU	ASP	H298	H298
R861	R861	T786	L715	Q639	VAL	VAL	D364	T299	T299
K862	K862	Y787	M716	D640	ARG	ARG	A365	I300	I300
Y865	Y865	C791	R721	K643	LEU	LEU	GLY	V301	V301
T866	T866	Y794	R722	V644	PRO	PRO	SER	E367	E367
N876	N876	Y794	E723	M645	ASN	ASN	LEU	Y302	Y302
V877	V877	T798	E723	M645	PRO	PRO	LEU	R303	R303
M878	M878	Y799	N724	F642	SER	SER	ASP	Y304	Y304
L879	L879	Y799	L725	P649	ALA	ALA	ASP	P305	P305
N880	N880	V803	K728	L652	ALA	ALA	SER	S370	S370
L881	L881	G804	L729		THR	THR	LEU	P371	P371
					PRO	PRO	SER	T372	T372
					ALA	ALA	SER	F373	F373
					THR	THR	LEU	V308	V308
					PRO	PRO	SER	X309	X309
					GLY	GLY	ASP	L310	L310
					SER	SER	LEU	H375	H375
					SER	SER	LEU	P376	P376
					SER	SER	SER	Q377	Q377
					SER	SER	ALA	S312	S312
					SER	SER	ALA	E313	E313

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.95Å 156.33Å 242.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.62 – 3.50 61.62 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.62-3.50) 99.5 (61.62-3.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.230 , 0.272 0.225 , 0.263	Depositor DCC
R_{free} test set	1313 reflections (5.17%)	DCC
Wilson B-factor (Å ²)	93.2	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 26700 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8967	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 093

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	0.61	1/4566 (0.0%)	0.84	1/6183 (0.0%)
1	B	0.48	0/4571	0.69	2/6189 (0.0%)
All	All	0.55	1/9137 (0.0%)	0.77	3/12372 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	864	CYS	CB-SG	-6.21	1.71	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	LYS	CD-CE-NZ	-5.49	99.07	111.70
1	A	818	LYS	N-CA-C	-5.24	96.86	111.00
1	B	710	LEU	CA-CB-CG	-5.02	103.75	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	589	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	591	ASN	Mainchain
1	A	663	THR	Mainchain
1	A	680	ALA	Peptide
1	A	737	THR	Mainchain
1	A	740	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	4457	0	4490	348	1
1	B	4462	0	4499	348	1
2	A	24	0	16	8	0
2	B	24	0	16	6	0
All	All	8967	0	9021	697	2

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 39.

All (697) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:HIS:CD2	1:A:377:GLN:H	1.54	1.24
1:B:311:SER:HB3	1:B:314:GLU:CB	1.76	1.15
1:B:299:THR:HB	1:B:303:ARG:HH11	1.10	1.14
1:A:705:GLN:HG2	1:A:890:VAL:HG13	1.22	1.13
1:A:629:THR:HB	1:A:672:LEU:HD12	1.18	1.10
1:A:421:PHE:HB3	1:A:422:PRO:HD2	1.33	1.10
1:A:322:ARG:HH12	1:A:353:MET:HG3	1.13	1.09
1:B:412:HIS:CE1	1:B:532:ASN:HB3	1.86	1.09
1:A:638:GLU:HG2	1:A:641:MET:HG3	1.32	1.09
1:A:629:THR:HB	1:A:672:LEU:CD1	1.86	1.05
1:A:298:HIS:HB3	1:A:302:TYR:CE1	1.91	1.04
1:A:591:ASN:O	1:A:595:ARG:HD3	1.58	1.04
1:A:645:ASN:HD22	1:A:645:ASN:C	1.62	1.01
1:A:299:THR:HA	1:A:302:TYR:CE2	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:SER:HB3	1:B:314:GLU:HB3	1.44	1.00
1:A:532:ASN:OD1	1:A:535:THR:HG23	1.63	0.99
1:B:408:GLU:HB3	1:B:409:ASP:HA	1.41	0.98
1:A:737:THR:HG22	1:A:738:SER:H	1.26	0.97
1:A:814:THR:HG23	1:A:818:LYS:H	1.27	0.97
1:B:702:ASP:HB3	1:B:739:SER:HA	1.47	0.95
1:B:570:GLU:CD	1:B:570:GLU:H	1.67	0.95
1:B:667:PRO:O	1:B:670:THR:HG22	1.65	0.95
1:A:830:ARG:HH22	1:A:903:LYS:NZ	1.64	0.95
1:A:335:PHE:HD2	1:A:335:PHE:C	1.69	0.95
1:A:319:TRP:CD1	1:A:323:PHE:HE2	1.84	0.95
1:A:375:HIS:HD2	1:A:377:GLN:N	1.63	0.95
1:B:329:LYS:NZ	1:B:361:ASP:H	1.64	0.94
1:A:734:VAL:HG22	1:A:744:LEU:HD23	1.48	0.94
1:B:654:PHE:HD1	1:B:655:PRO:HD2	1.33	0.93
1:A:561:GLU:CD	1:A:561:GLU:H	1.71	0.93
1:B:421:PHE:HB3	1:B:422:PRO:HD2	1.51	0.92
1:A:577:ALA:O	1:A:581:LYS:HD2	1.69	0.92
1:A:830:ARG:NH2	1:A:903:LYS:HZ1	1.68	0.92
1:B:710:LEU:CD2	1:B:732:TYR:O	2.18	0.92
1:B:634:LYS:HA	1:B:634:LYS:HE2	1.50	0.91
1:A:553:TRP:O	1:A:557:ILE:HG13	1.72	0.90
1:A:322:ARG:NH1	1:A:353:MET:HG3	1.86	0.90
1:A:591:ASN:OD1	1:A:592:PHE:N	2.05	0.90
1:B:710:LEU:HD23	1:B:732:TYR:O	1.72	0.90
1:B:739:SER:O	1:B:740:LYS:HG2	1.71	0.89
1:B:335:PHE:C	1:B:335:PHE:HD2	1.75	0.89
1:B:412:HIS:CE1	1:B:532:ASN:CB	2.54	0.89
1:A:830:ARG:HH22	1:A:903:LYS:HZ1	0.95	0.89
1:A:814:THR:CG2	1:A:818:LYS:H	1.84	0.89
1:B:827:ILE:HG23	1:B:828:LEU:HG	1.55	0.89
1:A:375:HIS:CD2	1:A:377:GLN:N	2.40	0.88
1:B:375:HIS:CD2	1:B:377:GLN:H	1.91	0.88
1:A:298:HIS:HB3	1:A:302:TYR:HE1	1.36	0.88
1:A:698:LYS:NZ	2:A:1949:093:CL	2.42	0.88
1:B:367:GLU:O	1:B:370:SER:OG	1.90	0.88
1:B:311:SER:HB3	1:B:314:GLU:HB2	1.52	0.88
1:A:319:TRP:CD1	1:A:323:PHE:CE2	2.60	0.88
1:A:654:PHE:HD1	1:A:655:PRO:HD2	1.40	0.87
1:B:332:LEU:CD1	1:B:336:LEU:HD11	2.03	0.87
1:A:363:GLU:HA	1:A:366:LEU:HD12	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:782:GLU:O	1:B:786:THR:HG23	1.74	0.86
1:B:299:THR:HB	1:B:303:ARG:NH1	1.88	0.86
1:A:335:PHE:CD2	1:A:335:PHE:C	2.44	0.86
1:B:678:MET:C	1:B:699:HIS:HE2	1.79	0.85
1:A:678:MET:O	1:A:699:HIS:CD2	2.30	0.84
1:A:647:THR:O	1:A:664:LYS:HB3	1.77	0.84
1:A:922:GLN:HE22	1:B:919:GLN:HB3	1.42	0.84
1:A:842:SER:OG	1:A:844:GLU:OE1	1.94	0.83
1:A:322:ARG:HD2	1:A:335:PHE:CD1	2.12	0.83
1:B:654:PHE:CD1	1:B:655:PRO:HD2	2.13	0.83
1:B:549:ASN:C	1:B:549:ASN:HD22	1.80	0.83
1:A:319:TRP:HE1	1:A:322:ARG:HH21	1.24	0.83
1:A:751:THR:HG22	1:A:754:GLU:HG3	1.61	0.83
1:A:335:PHE:CD1	1:A:357:TRP:CZ3	2.67	0.82
1:B:412:HIS:HE1	1:B:532:ASN:CB	1.92	0.82
1:B:876:ASN:HD22	1:B:876:ASN:H	1.27	0.81
1:B:296:GLN:O	1:B:300:ILE:HG22	1.81	0.81
1:B:654:PHE:HD1	1:B:655:PRO:CD	1.94	0.81
1:B:663:THR:OG1	1:B:664:LYS:HG2	1.81	0.81
1:A:705:GLN:CG	1:A:890:VAL:HG13	2.09	0.81
1:B:326:SER:HA	1:B:357:TRP:CZ2	2.16	0.80
1:B:329:LYS:HZ3	1:B:361:ASP:CG	1.84	0.80
1:B:712:MET:HE1	1:B:878:MET:HG2	1.64	0.80
1:B:734:VAL:HG22	1:B:744:LEU:HD22	1.61	0.80
1:B:749:SER:HB2	1:B:812:LEU:CD1	2.11	0.80
1:B:627:LYS:O	1:B:630:GLU:HG2	1.82	0.80
1:A:673:PHE:HB2	1:A:679:PRO:HD2	1.65	0.79
1:A:638:GLU:HG2	1:A:641:MET:CG	2.10	0.79
1:A:629:THR:CB	1:A:672:LEU:HD12	2.08	0.79
1:B:913:THR:HG23	1:B:916:GLU:HG3	1.65	0.79
1:B:332:LEU:HD12	1:B:336:LEU:HD11	1.65	0.78
1:A:591:ASN:O	1:A:595:ARG:CD	2.31	0.78
1:A:534:CYS:O	1:A:538:ILE:HG13	1.83	0.78
1:B:728:LYS:HD3	1:B:786:THR:HB	1.64	0.78
1:B:400:GLN:HE22	1:B:711:GLN:HE22	1.31	0.78
1:B:310:LEU:HD13	1:B:311:SER:OG	1.82	0.78
1:A:568:GLN:HA	1:A:568:GLN:OE1	1.83	0.78
1:A:737:THR:HG22	1:A:738:SER:N	1.99	0.77
1:A:645:ASN:ND2	1:A:645:ASN:C	2.35	0.77
1:A:294:ARG:HA	1:A:297:LEU:HD21	1.66	0.77
1:B:421:PHE:HB3	1:B:422:PRO:CD	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:HIS:HE1	1:A:318:VAL:HA	1.49	0.76
1:A:722:ARG:HH11	1:A:722:ARG:CG	1.98	0.76
1:A:322:ARG:NH1	1:A:335:PHE:HE1	1.83	0.76
1:A:678:MET:O	1:A:699:HIS:NE2	2.19	0.76
1:A:667:PRO:O	1:A:670:THR:HG23	1.85	0.75
1:B:315:GLN:HG3	1:B:338:CYS:HB2	1.67	0.75
1:A:322:ARG:HH11	1:A:335:PHE:HE1	1.33	0.75
1:B:791:CYS:SG	1:B:819:LEU:HD23	2.25	0.75
1:B:329:LYS:HZ2	1:B:361:ASP:H	1.34	0.75
1:B:631:LYS:O	1:B:635:LEU:HD23	1.85	0.75
1:B:329:LYS:NZ	1:B:361:ASP:CG	2.40	0.74
1:A:747:VAL:HG23	2:A:1949:093:HAK	1.52	0.74
1:A:807:HIS:H	1:A:810:ASN:HB2	1.50	0.74
1:A:410:PRO:O	1:A:414:VAL:HG23	1.88	0.74
1:B:335:PHE:CD2	1:B:335:PHE:C	2.52	0.74
1:A:677:LEU:HD11	1:A:700:GLY:H	1.50	0.74
1:A:706:ASP:O	1:A:710:LEU:HD12	1.87	0.74
1:B:332:LEU:HD22	1:B:357:TRP:HB3	1.69	0.74
1:A:626:ASN:HA	1:A:629:THR:CG2	2.18	0.74
1:B:302:TYR:HE2	1:B:303:ARG:HE	1.34	0.74
1:B:629:THR:O	1:B:633:GLN:HG3	1.87	0.73
1:A:843:LYS:O	1:A:847:GLU:HG3	1.88	0.73
1:B:329:LYS:HZ3	1:B:361:ASP:H	1.34	0.73
1:B:299:THR:CB	1:B:303:ARG:HH11	1.96	0.73
1:A:335:PHE:HD1	1:A:357:TRP:CH2	2.06	0.73
1:B:667:PRO:O	1:B:670:THR:CG2	2.35	0.73
1:B:703:LEU:HD13	1:B:744:LEU:HD21	1.71	0.73
1:B:311:SER:CB	1:B:314:GLU:HB3	2.18	0.73
1:A:319:TRP:NE1	1:A:323:PHE:CE2	2.57	0.73
1:A:405:LEU:HD23	1:A:533:LEU:HD21	1.68	0.73
1:B:948:ARG:O	1:B:949:LYS:HB2	1.87	0.73
1:A:639:GLN:NE2	1:A:645:ASN:OD1	2.22	0.73
1:A:375:HIS:HD2	1:A:377:GLN:H	0.87	0.72
1:A:638:GLU:CG	1:A:641:MET:HG3	2.16	0.72
1:A:322:ARG:HH12	1:A:353:MET:CG	1.96	0.72
1:A:421:PHE:HB3	1:A:422:PRO:CD	2.15	0.72
1:B:819:LEU:HD12	1:B:820:PHE:N	2.05	0.71
1:B:582:MET:O	1:B:586:VAL:HG23	1.90	0.71
1:B:738:SER:HB3	1:B:741:HIS:CE1	2.25	0.71
1:A:319:TRP:O	1:A:322:ARG:HB3	1.89	0.71
1:B:549:ASN:C	1:B:549:ASN:ND2	2.43	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LEU:HD13	1:A:377:GLN:HG2	1.70	0.71
1:B:335:PHE:HD1	1:B:357:TRP:CZ3	2.08	0.71
1:A:300:ILE:O	1:A:304:TYR:HB2	1.90	0.71
1:A:405:LEU:HD23	1:A:533:LEU:CD2	2.19	0.71
1:A:722:ARG:HH11	1:A:722:ARG:HG3	1.55	0.70
1:A:296:GLN:O	1:A:299:THR:HG22	1.92	0.70
1:B:319:TRP:HA	1:B:322:ARG:NE	2.06	0.70
1:B:749:SER:HB2	1:B:812:LEU:HD12	1.72	0.70
1:A:319:TRP:NE1	1:A:323:PHE:HE2	1.87	0.70
1:A:332:LEU:HD12	1:A:336:LEU:CD2	2.21	0.70
1:A:654:PHE:CD1	1:A:655:PRO:HD2	2.26	0.70
1:A:322:ARG:NH1	1:A:335:PHE:CE1	2.60	0.69
1:A:722:ARG:CB	1:A:722:ARG:HH11	2.05	0.69
1:B:678:MET:O	1:B:699:HIS:NE2	2.21	0.69
1:B:798:THR:HG23	1:B:803:VAL:HB	1.75	0.69
1:B:749:SER:CB	1:B:812:LEU:HD12	2.23	0.69
1:A:798:THR:HG23	1:A:803:VAL:HB	1.73	0.69
1:B:375:HIS:CD2	1:B:377:GLN:N	2.61	0.69
1:A:793:GLY:O	1:A:797:ILE:HG13	1.93	0.69
1:A:718:LYS:O	1:A:722:ARG:HG2	1.92	0.68
1:A:751:THR:HG22	1:A:754:GLU:CG	2.22	0.68
1:B:549:ASN:OD1	1:B:658:PRO:HG3	1.93	0.68
1:A:304:TYR:CB	1:A:305:PRO:HD3	2.24	0.68
1:B:314:GLU:O	1:B:318:VAL:HG12	1.93	0.68
1:A:329:LYS:HB3	1:A:360:MET:HA	1.75	0.68
1:A:913:THR:HG23	1:A:916:GLU:CD	2.13	0.68
1:A:322:ARG:HD2	1:A:335:PHE:CE1	2.27	0.68
1:B:297:LEU:HA	1:B:300:ILE:CG2	2.23	0.68
1:A:909:GLN:HG3	1:A:912:LEU:HG	1.75	0.68
1:A:332:LEU:HD12	1:A:336:LEU:HD23	1.74	0.68
1:B:335:PHE:HE2	1:B:339:ILE:HD13	1.58	0.68
1:B:751:THR:HA	1:B:812:LEU:HB3	1.75	0.67
1:A:629:THR:HA	1:A:672:LEU:HD11	1.76	0.67
1:A:769:HIS:CD2	1:A:815:THR:HG22	2.29	0.67
1:B:765:PHE:CD2	1:B:765:PHE:C	2.67	0.67
1:A:830:ARG:NH2	1:A:903:LYS:NZ	2.34	0.67
1:B:876:ASN:HD22	1:B:876:ASN:N	1.92	0.67
1:B:763:HIS:CD2	1:B:848:ALA:HA	2.29	0.67
1:A:654:PHE:HD1	1:A:655:PRO:CD	2.08	0.67
1:B:877:VAL:O	1:B:881:LEU:HG	1.95	0.67
1:B:578:MET:O	1:B:582:MET:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLN:HB2	1:B:338:CYS:HB3	1.77	0.67
1:B:549:ASN:ND2	1:B:553:TRP:CD1	2.63	0.67
1:A:625:ARG:O	1:A:629:THR:HG22	1.95	0.66
1:B:913:THR:HG23	1:B:916:GLU:CG	2.25	0.66
1:B:705:GLN:OE1	1:B:890:VAL:HG13	1.96	0.66
1:A:335:PHE:HD1	1:A:357:TRP:CZ3	2.13	0.66
1:B:297:LEU:HD23	1:B:297:LEU:H	1.60	0.66
1:A:343:LEU:HD13	1:A:345:ASP:H	1.61	0.66
1:A:326:SER:HB2	1:A:357:TRP:CE2	2.31	0.66
1:B:346:GLU:HA	1:B:349:GLN:CD	2.17	0.66
1:A:629:THR:CB	1:A:672:LEU:CD1	2.71	0.66
1:A:332:LEU:O	1:A:336:LEU:HD23	1.95	0.66
1:B:699:HIS:H	1:B:699:HIS:CD2	2.11	0.66
1:B:549:ASN:ND2	1:B:553:TRP:HD1	1.93	0.66
1:B:329:LYS:NZ	1:B:361:ASP:CB	2.59	0.65
1:A:294:ARG:HA	1:A:297:LEU:CD2	2.27	0.65
1:B:618:VAL:HG21	1:B:632:PHE:CD2	2.31	0.65
1:A:747:VAL:HG22	2:A:1949:093:HAE1	1.77	0.65
1:B:743:PHE:O	1:B:744:LEU:HD23	1.97	0.65
1:B:751:THR:HG23	1:B:754:GLU:H	1.59	0.65
1:B:749:SER:HB2	1:B:812:LEU:HD13	1.77	0.65
1:B:335:PHE:CD1	1:B:357:TRP:CZ3	2.84	0.65
1:A:362:VAL:O	1:A:365:ALA:HB3	1.97	0.65
1:B:827:ILE:CG2	1:B:828:LEU:HG	2.25	0.65
1:B:830:ARG:HH22	1:B:903:LYS:NZ	1.95	0.64
1:A:335:PHE:HD2	1:A:335:PHE:O	1.80	0.64
1:A:751:THR:CG2	1:A:754:GLU:H	2.10	0.64
1:B:319:TRP:CD1	1:B:319:TRP:C	2.71	0.64
1:A:363:GLU:HA	1:A:366:LEU:CD1	2.27	0.64
1:B:912:LEU:HD12	1:B:917:ALA:HA	1.78	0.64
1:A:785:ASP:OD1	1:A:789:LYS:HE3	1.98	0.64
1:A:405:LEU:CD2	1:A:533:LEU:HD21	2.28	0.64
1:B:329:LYS:HZ3	1:B:361:ASP:N	1.95	0.64
1:A:827:ILE:CG2	1:A:828:LEU:HG	2.28	0.64
1:A:751:THR:CG2	1:A:754:GLU:HG3	2.27	0.64
1:A:806:ARG:HA	1:A:810:ASN:HD22	1.62	0.64
1:A:862:LYS:O	1:A:866:THR:HG23	1.97	0.64
1:A:806:ARG:CZ	1:A:810:ASN:ND2	2.61	0.63
1:B:698:LYS:O	1:B:741:HIS:HA	1.98	0.63
1:B:610:GLU:CD	1:B:643:LYS:HG2	2.19	0.63
1:B:332:LEU:HD12	1:B:336:LEU:CD1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:GLU:CD	1:B:570:GLU:N	2.48	0.63
1:A:533:LEU:HD23	1:A:534:CYS:N	2.14	0.63
1:B:712:MET:CE	1:B:878:MET:HG2	2.28	0.63
1:B:812:LEU:HD21	1:B:822:ILE:HG21	1.81	0.63
1:A:866:THR:O	1:A:870:HIS:HD2	1.82	0.63
1:A:549:ASN:HD22	1:A:550:TYR:N	1.97	0.62
1:B:314:GLU:O	1:B:317:LEU:HG	1.99	0.62
1:B:329:LYS:NZ	1:B:361:ASP:N	2.43	0.62
1:A:811:LEU:C	1:A:812:LEU:HD23	2.18	0.62
1:A:813:LEU:HD12	1:A:818:LYS:O	1.98	0.62
1:B:621:GLU:HG2	1:B:623:GLY:H	1.63	0.62
1:A:319:TRP:HD1	1:A:323:PHE:CE2	2.17	0.62
1:B:806:ARG:NH1	1:B:823:ASP:O	2.29	0.62
1:A:677:LEU:HD21	1:A:699:HIS:HB2	1.80	0.62
1:A:657:ASP:C	1:A:657:ASP:OD2	2.37	0.62
1:B:319:TRP:HD1	1:B:319:TRP:O	1.82	0.62
1:A:363:GLU:CA	1:A:366:LEU:HD12	2.29	0.62
1:B:751:THR:HG22	1:B:754:GLU:HB2	1.82	0.62
1:B:749:SER:CB	1:B:812:LEU:CD1	2.76	0.62
1:A:664:LYS:H	1:A:685:VAL:CG2	2.12	0.62
1:A:578:MET:O	1:A:582:MET:HG3	2.00	0.61
1:B:411:ARG:HA	1:B:414:VAL:HG22	1.81	0.61
1:B:826:TYR:HB3	1:B:830:ARG:O	2.00	0.61
1:B:549:ASN:HD21	1:B:553:TRP:HD1	1.46	0.61
1:B:751:THR:HG22	1:B:754:GLU:CG	2.31	0.61
1:A:813:LEU:CD1	1:A:818:LYS:O	2.49	0.61
1:B:913:THR:HG23	1:B:916:GLU:CD	2.21	0.61
1:A:723:GLU:O	1:A:724:ASN:HB3	1.99	0.61
1:A:335:PHE:CD1	1:A:357:TRP:HZ3	2.17	0.60
1:A:580:LEU:HD22	1:A:581:LYS:HE2	1.82	0.60
1:A:803:VAL:HG12	1:A:806:ARG:HD3	1.83	0.60
1:A:689:ALA:HB3	1:A:691:HIS:CE1	2.34	0.60
1:A:580:LEU:HD22	1:A:581:LYS:CE	2.32	0.60
1:B:703:LEU:CD1	1:B:744:LEU:HD21	2.31	0.60
1:A:716:MET:SD	1:A:797:ILE:HG23	2.42	0.60
1:A:812:LEU:HD11	1:A:822:ILE:CD1	2.31	0.60
1:B:618:VAL:HG21	1:B:632:PHE:HD2	1.66	0.60
1:A:549:ASN:ND2	1:A:549:ASN:C	2.54	0.60
1:A:315:GLN:HG3	1:A:316:ASP:OD2	2.01	0.60
1:B:587:LEU:HB3	1:B:598:PHE:HB2	1.84	0.60
1:B:315:GLN:HG2	1:B:316:ASP:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:THR:HG22	1:A:754:GLU:CB	2.31	0.60
1:B:749:SER:OG	2:B:1950:093:NAR	2.35	0.60
1:B:722:ARG:HH11	1:B:722:ARG:HB3	1.66	0.60
1:B:412:HIS:HE1	1:B:532:ASN:HB2	1.64	0.60
1:A:722:ARG:HG3	1:A:722:ARG:NH1	2.17	0.60
1:B:807:HIS:CD2	1:B:809:ASP:HB2	2.36	0.60
1:A:649:PHE:HE1	1:A:662:ILE:HG13	1.66	0.60
1:B:339:ILE:O	1:B:342:LYS:HB3	2.01	0.60
1:B:629:THR:HG22	1:B:672:LEU:HB3	1.84	0.60
1:B:573:HIS:C	1:B:573:HIS:CD2	2.75	0.59
1:A:806:ARG:CZ	1:A:810:ASN:HD22	2.14	0.59
1:A:920:HIS:CD2	1:A:920:HIS:C	2.75	0.59
1:B:645:ASN:C	1:B:645:ASN:OD1	2.40	0.59
1:A:297:LEU:O	1:A:301:VAL:HG23	2.03	0.59
1:B:614:LEU:HD21	1:B:636:LEU:HD23	1.84	0.59
1:B:335:PHE:CD1	1:B:357:TRP:HZ3	2.21	0.59
1:A:709:ILE:HD12	1:A:801:LEU:HD13	1.83	0.59
1:B:412:HIS:NE2	1:B:532:ASN:HB3	2.18	0.58
1:A:645:ASN:HD22	1:A:646:PHE:N	2.01	0.58
1:B:814:THR:OG1	1:B:816:ASN:HB3	2.03	0.58
1:A:335:PHE:CD1	1:A:357:TRP:CH2	2.88	0.58
1:A:812:LEU:HD11	1:A:822:ILE:HD12	1.84	0.58
1:A:406:LYS:NZ	1:A:887:ASP:O	2.36	0.58
1:B:319:TRP:HA	1:B:322:ARG:HE	1.66	0.58
1:B:614:LEU:C	1:B:614:LEU:HD12	2.24	0.58
1:B:862:LYS:O	1:B:866:THR:HG22	2.03	0.58
1:B:599:TYR:O	1:B:599:TYR:HD2	1.87	0.58
1:B:799:TYR:O	1:B:907:ASN:ND2	2.37	0.58
1:A:363:GLU:N	1:A:363:GLU:CD	2.57	0.58
1:B:710:LEU:HD22	1:B:732:TYR:O	2.03	0.58
1:A:305:PRO:O	1:A:334:LYS:NZ	2.37	0.58
1:B:812:LEU:HD12	1:B:820:PHE:CZ	2.39	0.57
1:A:373:PHE:CD2	1:A:373:PHE:N	2.71	0.57
1:B:634:LYS:CE	1:B:634:LYS:HA	2.21	0.57
1:A:657:ASP:OD2	1:A:659:GLU:N	2.37	0.57
1:B:544:ASN:OD1	1:B:544:ASN:C	2.42	0.57
1:A:538:ILE:HG23	1:A:583:PHE:HD1	1.69	0.57
1:B:830:ARG:NH2	1:B:903:LYS:NZ	2.52	0.57
1:A:621:GLU:O	1:A:628:LYS:HE2	2.04	0.57
1:B:392:GLU:HG2	1:B:393:ASP:N	2.19	0.57
1:B:375:HIS:NE2	1:B:377:GLN:HB2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:HIS:HD2	1:A:809:ASP:HB2	1.70	0.57
1:A:373:PHE:HD2	1:A:373:PHE:N	2.02	0.57
1:B:841:LEU:O	1:B:932:VAL:HG21	2.05	0.57
1:A:335:PHE:CD2	1:A:335:PHE:O	2.57	0.57
1:A:865:TYR:HD1	1:A:921:LEU:HD23	1.69	0.57
1:A:319:TRP:HE1	1:A:322:ARG:NH2	2.00	0.56
1:B:590:GLY:O	1:B:595:ARG:HD3	2.05	0.56
1:A:421:PHE:CB	1:A:422:PRO:HD2	2.22	0.56
1:A:677:LEU:HD11	1:A:700:GLY:N	2.20	0.56
1:A:898:ASP:OD1	1:A:898:ASP:N	2.37	0.56
1:B:344:GLU:O	1:B:347:VAL:HB	2.04	0.56
1:B:702:ASP:HB3	1:B:739:SER:CA	2.30	0.56
1:B:878:MET:O	1:B:882:PHE:HD2	1.88	0.56
1:A:375:HIS:HB3	1:A:378:VAL:HG22	1.88	0.56
1:B:332:LEU:O	1:B:336:LEU:HD22	2.06	0.56
1:A:326:SER:HB2	1:A:357:TRP:NE1	2.20	0.56
1:B:723:GLU:O	1:B:724:ASN:OD1	2.24	0.56
1:B:416:LEU:O	1:B:420:ILE:HG12	2.06	0.56
1:B:318:VAL:HG23	1:B:322:ARG:HB2	1.88	0.56
1:B:335:PHE:HD1	1:B:357:TRP:HZ3	1.50	0.56
1:A:335:PHE:CE1	1:A:357:TRP:HZ3	2.24	0.56
1:B:400:GLN:HE22	1:B:711:GLN:NE2	2.02	0.56
1:A:415:HIS:ND1	1:A:415:HIS:C	2.59	0.56
1:A:417:HIS:ND1	1:A:417:HIS:C	2.58	0.56
1:B:934:PRO:O	1:B:938:GLU:HG3	2.06	0.56
1:B:763:HIS:NE2	1:B:848:ALA:HA	2.21	0.55
1:B:876:ASN:N	1:B:876:ASN:ND2	2.54	0.55
1:B:649:PHE:CE2	1:B:664:LYS:HA	2.41	0.55
1:B:329:LYS:HZ3	1:B:361:ASP:CB	2.19	0.55
1:A:409:ASP:OD1	1:A:411:ARG:N	2.39	0.55
1:A:827:ILE:HG23	1:A:828:LEU:HG	1.87	0.55
1:B:402:VAL:O	1:B:405:LEU:HB2	2.05	0.55
1:B:343:LEU:O	1:B:346:GLU:HG2	2.07	0.55
1:A:869:LEU:HD11	1:A:918:VAL:CG2	2.36	0.55
1:B:325:LEU:O	1:B:327:SER:N	2.40	0.55
1:B:343:LEU:HG	1:B:344:GLU:H	1.71	0.55
1:A:405:LEU:CD2	1:A:533:LEU:CD2	2.85	0.55
1:B:806:ARG:HD2	1:B:806:ARG:N	2.22	0.55
1:B:333:THR:HA	1:B:336:LEU:CD2	2.38	0.54
1:A:772:CYS:O	1:A:778:GLY:HA2	2.07	0.54
1:A:409:ASP:HB3	1:A:412:HIS:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLN:CG	1:B:338:CYS:HB2	2.35	0.54
1:B:299:THR:O	1:B:302:TYR:HD2	1.90	0.54
1:A:751:THR:HG22	1:A:754:GLU:H	1.72	0.54
1:A:930:THR:HA	1:A:936:LEU:HD12	1.90	0.54
1:A:629:THR:CA	1:A:672:LEU:HD11	2.37	0.54
1:A:645:ASN:ND2	1:A:647:THR:H	2.06	0.54
1:B:712:MET:O	1:B:716:MET:HG3	2.07	0.54
1:B:640:ASP:OD1	1:B:640:ASP:C	2.46	0.54
1:A:645:ASN:ND2	1:A:647:THR:N	2.56	0.53
1:A:391:ASP:CG	1:A:540:ARG:HH12	2.10	0.53
1:B:366:LEU:HD12	1:B:881:LEU:HD21	1.91	0.53
1:A:610:GLU:HG3	1:A:644:VAL:HG12	1.90	0.53
1:B:375:HIS:C	1:B:375:HIS:CD2	2.82	0.53
1:A:677:LEU:O	1:A:679:PRO:HD3	2.08	0.53
1:B:767:ARG:O	1:B:771:PRO:HG3	2.09	0.53
1:A:811:LEU:O	1:A:812:LEU:HD23	2.09	0.53
1:A:304:TYR:HB2	1:A:305:PRO:HD3	1.89	0.53
1:A:806:ARG:HA	1:A:810:ASN:ND2	2.23	0.53
1:A:807:HIS:HA	1:B:947:TRP:CZ3	2.44	0.53
1:B:765:PHE:HD2	1:B:766:PHE:N	2.06	0.53
1:A:705:GLN:HG3	1:A:891:PRO:HD2	1.91	0.53
1:B:408:GLU:HB3	1:B:409:ASP:CA	2.29	0.52
1:B:766:PHE:CE1	1:B:817:GLY:HA2	2.44	0.52
1:A:375:HIS:O	1:A:378:VAL:HG23	2.09	0.52
1:B:744:LEU:HD13	2:B:1950:093:CAC	2.39	0.52
1:A:575:MET:C	1:A:575:MET:SD	2.88	0.52
1:A:319:TRP:O	1:A:319:TRP:HD1	1.92	0.52
1:A:723:GLU:O	1:A:724:ASN:CB	2.58	0.52
1:A:567:LYS:HG3	1:A:568:GLN:H	1.75	0.52
1:B:412:HIS:CE1	1:B:532:ASN:HB2	2.39	0.52
1:B:621:GLU:O	1:B:628:LYS:HE2	2.09	0.52
1:B:552:TYR:CG	1:B:601:LEU:HD13	2.45	0.51
1:A:645:ASN:ND2	1:A:648:ASN:H	2.08	0.51
1:A:649:PHE:CE1	1:A:663:THR:O	2.64	0.51
1:A:626:ASN:HA	1:A:629:THR:HG22	1.89	0.51
1:B:371:PRO:HB3	1:B:407:TYR:CE2	2.45	0.51
1:A:763:HIS:NE2	1:A:848:ALA:O	2.35	0.51
2:A:1949:093:CAE	2:A:1949:093:HAD	2.40	0.51
1:A:689:ALA:O	1:A:690:HIS:HB2	2.10	0.51
1:B:315:GLN:HA	1:B:318:VAL:HG13	1.93	0.51
1:B:751:THR:HG22	1:B:754:GLU:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:ASP:OD2	1:B:657:ASP:C	2.49	0.51
2:A:1949:093:SAP	2:A:1949:093:OAL	2.69	0.51
1:B:552:TYR:OH	1:B:605:ARG:NE	2.36	0.51
1:A:944:THR:OG1	1:B:931:ALA:O	2.26	0.51
1:A:375:HIS:HB3	1:A:378:VAL:CG2	2.41	0.51
2:B:1950:093:SAP	2:B:1950:093:CAT	2.99	0.51
1:B:909:GLN:HB3	1:B:912:LEU:HG	1.93	0.51
1:B:843:LYS:HA	1:B:932:VAL:HG13	1.92	0.51
1:A:764:ASN:OD1	1:A:767:ARG:NH1	2.44	0.51
1:A:367:GLU:O	1:A:370:SER:HB3	2.10	0.51
1:B:830:ARG:HH22	1:B:903:LYS:CE	2.24	0.51
1:B:312:SER:HA	1:B:315:GLN:OE1	2.10	0.50
1:B:409:ASP:OD1	1:B:410:PRO:HD2	2.12	0.50
1:A:609:ASP:O	1:A:613:LYS:HG3	2.11	0.50
1:B:828:LEU:O	1:B:830:ARG:NH1	2.44	0.50
1:A:722:ARG:CG	1:A:722:ARG:NH1	2.66	0.50
1:A:305:PRO:HB2	1:A:308:TYR:CD2	2.46	0.50
1:B:807:HIS:NE2	1:B:809:ASP:HB2	2.27	0.50
1:B:345:ASP:O	1:B:349:GLN:HG3	2.11	0.50
1:B:634:LYS:CA	1:B:634:LYS:HE2	2.33	0.50
1:B:375:HIS:HD2	1:B:377:GLN:N	2.10	0.50
1:A:807:HIS:HA	1:B:947:TRP:HZ3	1.77	0.50
1:B:807:HIS:HD2	1:B:809:ASP:H	1.59	0.50
1:A:661:TYR:HB2	1:A:687:SER:HB3	1.92	0.50
1:B:677:LEU:HD11	1:B:700:GLY:HA3	1.93	0.50
1:B:318:VAL:O	1:B:322:ARG:N	2.39	0.50
1:A:696:ILE:HG22	1:A:697:PHE:N	2.25	0.50
1:A:807:HIS:CD2	1:A:809:ASP:HB2	2.46	0.50
1:A:872:ARG:HH12	1:A:909:GLN:C	2.14	0.50
1:A:722:ARG:HB2	1:A:722:ARG:HH11	1.75	0.50
1:B:629:THR:HG22	1:B:672:LEU:CB	2.41	0.50
1:B:806:ARG:HB3	1:B:811:LEU:HD21	1.94	0.50
1:B:673:PHE:HB2	1:B:679:PRO:HD2	1.93	0.50
1:A:827:ILE:HG22	1:A:828:LEU:HG	1.94	0.49
1:B:569:ASP:C	1:B:569:ASP:OD1	2.51	0.49
1:A:544:ASN:OD1	1:A:546:THR:N	2.45	0.49
1:A:360:MET:HE1	1:A:365:ALA:HA	1.95	0.49
1:B:876:ASN:H	1:B:876:ASN:ND2	2.01	0.49
1:B:399:LEU:H	1:B:399:LEU:HD22	1.76	0.49
1:A:360:MET:HG2	1:A:364:ASP:HB2	1.93	0.49
1:A:751:THR:HG23	1:A:754:GLU:H	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1950:093:CL	2:B:1950:093:NAU	2.81	0.49
1:A:409:ASP:OD1	1:A:409:ASP:C	2.50	0.49
1:B:321:PHE:O	1:B:325:LEU:HD23	2.12	0.49
1:B:297:LEU:HA	1:B:300:ILE:HG22	1.94	0.49
1:B:329:LYS:O	1:B:332:LEU:HB3	2.12	0.49
1:B:894:ALA:O	1:B:897:PRO:HD3	2.13	0.49
1:B:339:ILE:HD12	1:B:350:ALA:CB	2.42	0.49
1:A:872:ARG:NH1	1:A:909:GLN:O	2.44	0.49
1:B:599:TYR:O	1:B:603:LYS:HG3	2.13	0.49
1:B:590:GLY:HA3	1:B:594:LEU:HB2	1.94	0.49
1:B:577:ALA:O	1:B:581:LYS:HD3	2.13	0.49
1:B:335:PHE:O	1:B:335:PHE:HD2	1.94	0.48
1:B:346:GLU:HA	1:B:349:GLN:OE1	2.13	0.48
1:B:300:ILE:O	1:B:304:TYR:HD2	1.95	0.48
1:A:806:ARG:N	1:A:806:ARG:HD2	2.28	0.48
1:A:399:LEU:HB3	1:A:400:GLN:NE2	2.28	0.48
1:B:299:THR:O	1:B:302:TYR:CD2	2.66	0.48
2:B:1950:093:HAT2	2:B:1950:093:SAP	2.53	0.48
1:B:413:ILE:HD13	1:B:575:MET:HG2	1.95	0.48
1:B:329:LYS:NZ	1:B:361:ASP:HB2	2.27	0.48
1:B:648:ASN:HA	1:B:664:LYS:HB3	1.96	0.48
1:A:843:LYS:HA	1:A:932:VAL:CG1	2.43	0.48
1:B:310:LEU:HD22	1:B:311:SER:H	1.78	0.48
1:B:357:TRP:CD1	1:B:358:ALA:N	2.81	0.48
1:A:807:HIS:O	1:A:810:ASN:HB2	2.13	0.48
1:A:786:THR:O	1:A:790:SER:OG	2.29	0.48
1:B:300:ILE:HA	1:B:304:TYR:CD2	2.49	0.48
1:B:399:LEU:H	1:B:399:LEU:CD2	2.27	0.48
1:B:906:GLU:O	1:B:909:GLN:NE2	2.47	0.48
1:A:769:HIS:HB3	1:A:770:HIS:HD2	1.78	0.48
1:B:823:ASP:OD1	1:B:824:PHE:N	2.46	0.48
1:B:382:ALA:O	1:B:385:ARG:HB2	2.14	0.48
1:B:783:VAL:HG13	1:B:816:ASN:O	2.14	0.48
1:A:561:GLU:N	1:A:561:GLU:CD	2.53	0.48
1:A:544:ASN:OD1	1:A:544:ASN:C	2.52	0.48
1:B:388:GLN:HA	1:B:388:GLN:OE1	2.13	0.48
1:B:656:LEU:C	1:B:656:LEU:HD23	2.34	0.48
1:B:888:ALA:O	1:B:889:THR:HG22	2.14	0.48
1:A:729:LEU:HD21	1:A:793:GLY:HA3	1.96	0.48
1:A:737:THR:HB	1:A:741:HIS:CD2	2.48	0.47
1:B:567:LYS:C	1:B:570:GLU:OE1	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:VAL:O	1:B:305:PRO:HD2	2.14	0.47
1:A:608:ILE:HG21	1:A:737:THR:HG21	1.96	0.47
1:A:614:LEU:HD21	1:A:636:LEU:CD2	2.44	0.47
1:B:752:VAL:HG12	1:B:808:LEU:HD23	1.96	0.47
1:B:555:LEU:HB3	1:B:580:LEU:HG	1.96	0.47
1:A:776:PRO:HD2	1:A:779:ILE:O	2.14	0.47
1:B:364:ASP:O	1:B:367:GLU:HB3	2.14	0.47
1:A:308:TYR:CD1	1:A:310:LEU:HD13	2.49	0.47
1:A:399:LEU:HB3	1:A:400:GLN:HE22	1.78	0.47
1:A:737:THR:CG2	1:A:741:HIS:CD2	2.98	0.47
1:A:790:SER:CB	1:A:819:LEU:H	2.27	0.47
1:B:598:PHE:C	1:B:598:PHE:CD2	2.87	0.47
1:A:329:LYS:HG3	1:A:329:LYS:H	1.32	0.47
1:A:614:LEU:HD21	1:A:636:LEU:HD23	1.96	0.47
1:B:322:ARG:HG3	1:B:335:PHE:CD1	2.50	0.47
1:A:737:THR:CG2	1:A:738:SER:N	2.69	0.47
1:B:312:SER:O	1:B:315:GLN:HG2	2.14	0.47
1:B:408:GLU:CB	1:B:409:ASP:HA	2.18	0.47
1:A:343:LEU:HD13	1:A:345:ASP:N	2.28	0.47
1:B:717:ASP:HB2	1:B:729:LEU:HD12	1.97	0.47
1:B:879:LEU:HD23	1:B:879:LEU:N	2.29	0.47
1:B:777:TYR:CD1	1:B:777:TYR:N	2.83	0.47
1:B:329:LYS:HZ1	1:B:361:ASP:HB2	1.79	0.46
1:A:332:LEU:HD12	1:A:336:LEU:HD21	1.93	0.46
1:A:747:VAL:CG2	2:A:1949:093:HAK	2.25	0.46
1:A:915:GLU:OE2	1:A:915:GLU:N	2.46	0.46
1:B:696:ILE:O	1:B:743:PHE:HA	2.15	0.46
1:A:291:ALA:O	1:A:294:ARG:NE	2.48	0.46
1:B:697:PHE:HA	1:B:742:GLY:O	2.16	0.46
1:A:402:VAL:O	1:A:405:LEU:HB2	2.15	0.46
1:A:827:ILE:N	1:A:892:ASP:OD2	2.39	0.46
1:B:354:LEU:HD23	1:B:354:LEU:C	2.35	0.46
1:A:708:LEU:HD12	1:A:890:VAL:HG21	1.97	0.46
1:A:814:THR:CG2	1:A:818:LYS:N	2.66	0.46
1:B:678:MET:HA	1:B:679:PRO:HD3	1.63	0.46
1:A:303:ARG:O	1:A:304:TYR:CD2	2.69	0.46
1:B:764:ASN:HA	1:B:767:ARG:NH1	2.30	0.46
1:B:319:TRP:CG	1:B:322:ARG:CZ	2.98	0.46
1:A:708:LEU:O	1:A:708:LEU:HD23	2.15	0.46
1:A:922:GLN:HE22	1:B:919:GLN:CB	2.21	0.46
1:B:948:ARG:O	1:B:949:LYS:CB	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:HIS:CD2	1:A:376:PRO:N	2.83	0.46
1:A:298:HIS:CE1	1:A:318:VAL:HA	2.39	0.46
1:B:752:VAL:CG1	1:B:808:LEU:HD23	2.46	0.46
1:A:590:GLY:HA3	1:A:594:LEU:HD12	1.98	0.46
1:A:654:PHE:HB3	1:A:657:ASP:O	2.16	0.46
1:B:642:PHE:HB2	1:B:644:VAL:O	2.16	0.46
1:B:788:ILE:HG13	1:B:860:PHE:HB2	1.96	0.46
1:B:367:GLU:O	1:B:367:GLU:HG3	2.14	0.46
1:B:763:HIS:NE2	1:B:848:ALA:O	2.49	0.46
1:A:649:PHE:CD1	1:A:663:THR:O	2.69	0.46
1:A:391:ASP:CG	1:A:540:ARG:NH1	2.68	0.46
1:B:302:TYR:CZ	1:B:303:ARG:HG3	2.50	0.46
1:A:332:LEU:HD23	1:A:360:MET:HB2	1.98	0.46
1:A:408:GLU:OE2	1:A:533:LEU:N	2.48	0.46
1:B:776:PRO:HG2	1:B:777:TYR:H	1.81	0.46
1:B:756:LEU:HA	1:B:759:GLU:O	2.16	0.46
1:B:891:PRO:O	1:B:895:LEU:HD12	2.14	0.46
1:A:375:HIS:C	1:A:375:HIS:CD2	2.88	0.46
1:A:629:THR:HB	1:A:672:LEU:HD11	1.90	0.46
1:B:625:ARG:HG3	1:B:672:LEU:HD22	1.97	0.46
1:B:360:MET:O	1:B:385:ARG:NH2	2.48	0.46
1:B:664:LYS:HG3	1:B:685:VAL:HG23	1.98	0.45
1:A:785:ASP:O	1:A:789:LYS:HG3	2.16	0.45
1:B:544:ASN:OD1	1:B:547:LEU:HB2	2.16	0.45
1:A:319:TRP:NE1	1:A:322:ARG:NH2	2.53	0.45
1:B:899:LYS:O	1:B:903:LYS:HG3	2.16	0.45
1:B:594:LEU:N	1:B:594:LEU:HD23	2.30	0.45
1:A:363:GLU:H	1:A:363:GLU:CD	2.18	0.45
1:B:366:LEU:HD12	1:B:881:LEU:CD2	2.46	0.45
1:A:814:THR:CG2	1:A:818:LYS:HB2	2.47	0.45
1:A:319:TRP:CD1	1:A:322:ARG:NE	2.74	0.45
1:A:734:VAL:CG2	1:A:744:LEU:HD23	2.34	0.45
1:A:878:MET:HA	1:A:881:LEU:HD12	1.99	0.45
1:B:339:ILE:CD1	1:B:350:ALA:HB1	2.46	0.45
1:B:939:GLN:HG2	1:B:943:PHE:CZ	2.52	0.45
1:B:710:LEU:O	1:B:714:THR:OG1	2.34	0.45
1:A:718:LYS:O	1:A:722:ARG:CG	2.63	0.45
1:A:723:GLU:OE1	1:A:723:GLU:N	2.50	0.45
1:B:314:GLU:O	1:B:318:VAL:CG1	2.61	0.45
1:B:357:TRP:HD1	1:B:358:ALA:N	2.15	0.45
1:B:821:HIS:CD2	1:B:821:HIS:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:CD1	1:A:336:LEU:HD21	2.47	0.45
1:A:553:TRP:O	1:A:557:ILE:CG1	2.55	0.45
1:A:689:ALA:CB	1:A:691:HIS:CE1	2.99	0.44
1:A:782:GLU:O	1:A:786:THR:HG23	2.17	0.44
1:B:664:LYS:HG3	1:B:685:VAL:CG2	2.47	0.44
1:A:549:ASN:C	1:A:549:ASN:HD22	2.18	0.44
1:A:783:VAL:HG13	1:A:816:ASN:O	2.17	0.44
1:B:747:VAL:HG12	2:B:1950:093:HAE1	2.00	0.44
1:B:794:TYR:CD1	1:B:821:HIS:CD2	3.05	0.44
1:B:308:TYR:HD2	1:B:308:TYR:HA	1.69	0.44
1:A:649:PHE:CE1	1:A:662:ILE:HG13	2.48	0.44
1:A:335:PHE:HE2	1:A:339:ILE:HD12	1.81	0.44
1:B:366:LEU:CD1	1:B:881:LEU:HD21	2.47	0.44
1:A:896:GLU:OE1	1:A:898:ASP:OD1	2.36	0.44
1:B:739:SER:O	1:B:740:LYS:CG	2.56	0.44
1:B:699:HIS:N	1:B:699:HIS:CD2	2.82	0.44
1:A:709:ILE:O	1:A:712:MET:HB2	2.17	0.44
1:A:397:TYR:O	1:A:398:LEU:C	2.56	0.44
1:A:759:GLU:O	1:A:760:GLY:C	2.56	0.44
1:B:302:TYR:CE2	1:B:303:ARG:HG3	2.52	0.44
1:A:747:VAL:HG23	2:A:1949:093:NAK	2.26	0.44
1:A:719:LEU:O	1:A:723:GLU:HG2	2.17	0.44
1:B:600:ASN:HA	1:B:603:LYS:HD3	2.00	0.44
1:B:636:LEU:HD12	1:B:670:THR:HG21	2.00	0.43
1:B:766:PHE:HE1	1:B:817:GLY:HA2	1.83	0.43
1:B:664:LYS:HE3	1:B:685:VAL:HG21	2.01	0.43
1:A:811:LEU:HD23	1:A:811:LEU:N	2.33	0.43
1:A:395:LEU:C	1:A:395:LEU:HD23	2.38	0.43
1:A:328:HIS:O	1:A:331:ALA:HB3	2.17	0.43
1:A:532:ASN:ND2	1:A:534:CYS:SG	2.89	0.43
1:A:396:LEU:HD12	1:A:718:LYS:HE3	2.00	0.43
1:B:325:LEU:C	1:B:327:SER:N	2.71	0.43
1:B:865:TYR:OH	1:B:922:GLN:HG3	2.17	0.43
1:B:310:LEU:HD13	1:B:311:SER:HG	1.83	0.43
1:B:350:ALA:O	1:B:354:LEU:N	2.44	0.43
1:A:625:ARG:HG3	1:A:626:ASN:N	2.27	0.43
1:A:319:TRP:NE1	1:A:323:PHE:CZ	2.85	0.43
1:B:375:HIS:O	1:B:378:VAL:HG22	2.18	0.43
1:B:368:LEU:C	1:B:370:SER:H	2.22	0.43
1:A:668:MET:N	1:A:668:MET:SD	2.85	0.43
1:A:888:ALA:O	1:A:889:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:THR:OG1	1:B:691:HIS:HB2	2.18	0.43
1:A:344:GLU:O	1:A:348:THR:HG23	2.18	0.43
1:A:723:GLU:OE1	1:A:723:GLU:CA	2.67	0.43
1:B:575:MET:O	1:B:579:VAL:HG23	2.18	0.43
1:A:652:ILE:HG22	1:A:653:PRO:O	2.19	0.43
1:B:704:ARG:H	1:B:704:ARG:HG3	1.60	0.43
1:B:311:SER:HB3	1:B:314:GLU:CD	2.39	0.43
1:A:547:LEU:HD23	1:A:547:LEU:HA	1.85	0.43
1:B:370:SER:HB3	1:B:371:PRO:HD2	2.01	0.43
1:A:822:ILE:HD13	1:A:822:ILE:HG21	1.77	0.43
1:A:865:TYR:CD1	1:A:921:LEU:HD23	2.52	0.43
1:A:381:TYR:O	1:A:385:ARG:HG2	2.18	0.43
1:B:368:LEU:HD22	1:B:373:PHE:CE2	2.54	0.43
1:A:684:PHE:O	1:A:692:GLU:HA	2.17	0.43
1:B:343:LEU:CG	1:B:344:GLU:H	2.31	0.43
1:A:335:PHE:HD2	1:A:336:LEU:N	2.15	0.43
1:A:391:ASP:N	1:A:391:ASP:OD2	2.52	0.43
1:B:893:ILE:O	1:B:897:PRO:HA	2.18	0.43
1:B:888:ALA:O	1:B:889:THR:CB	2.67	0.43
1:A:908:LEU:HA	1:A:908:LEU:HD23	1.81	0.43
1:A:641:MET:HE2	1:A:642:PHE:CE1	2.54	0.42
1:A:820:PHE:CD2	1:A:820:PHE:N	2.87	0.42
1:B:300:ILE:HA	1:B:304:TYR:HD2	1.84	0.42
1:B:300:ILE:HG12	1:B:304:TYR:CD2	2.54	0.42
1:A:845:MET:O	1:A:848:ALA:HB3	2.19	0.42
1:A:843:LYS:HE2	1:A:847:GLU:OE2	2.18	0.42
1:B:717:ASP:OD1	1:B:721:ARG:HG3	2.19	0.42
1:A:602:ARG:NH1	1:A:606:ARG:HD2	2.33	0.42
1:A:830:ARG:NH1	1:A:903:LYS:HZ2	2.17	0.42
1:A:673:PHE:HE2	1:A:696:ILE:HG12	1.84	0.42
1:B:912:LEU:HB3	1:B:916:GLU:HB2	2.00	0.42
1:B:837:PRO:O	1:B:840:LYS:HE3	2.19	0.42
1:B:611:LEU:HG	1:B:646:PHE:CE2	2.54	0.42
1:A:826:TYR:HB3	1:A:830:ARG:O	2.20	0.42
1:A:830:ARG:HH12	1:A:903:LYS:HZ2	1.66	0.42
1:B:656:LEU:HD23	1:B:657:ASP:N	2.35	0.42
1:B:314:GLU:HA	1:B:317:LEU:HD23	2.02	0.42
1:B:329:LYS:HZ1	1:B:361:ASP:CB	2.32	0.42
1:B:614:LEU:HD21	1:B:636:LEU:CD2	2.47	0.42
1:A:823:ASP:O	1:A:823:ASP:CG	2.58	0.42
1:A:580:LEU:HD23	1:A:584:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:LEU:O	1:A:932:VAL:HG21	2.20	0.42
1:B:741:HIS:ND1	1:B:741:HIS:N	2.68	0.42
1:A:860:PHE:CE1	1:A:864:CYS:SG	3.13	0.42
1:B:570:GLU:OE1	1:B:570:GLU:N	2.51	0.41
1:B:375:HIS:CD2	1:B:376:PRO:N	2.88	0.41
1:A:747:VAL:HG21	1:A:820:PHE:CZ	2.55	0.41
1:A:400:GLN:N	1:A:400:GLN:NE2	2.68	0.41
1:A:375:HIS:NE2	1:A:377:GLN:CB	2.84	0.41
1:A:923:SER:O	1:A:927:VAL:HG22	2.20	0.41
1:A:405:LEU:HA	1:A:405:LEU:HD23	1.75	0.41
1:B:375:HIS:NE2	1:B:377:GLN:CB	2.82	0.41
1:B:743:PHE:C	1:B:744:LEU:HD23	2.40	0.41
1:A:403:GLN:NE2	1:A:888:ALA:HA	2.35	0.41
1:A:319:TRP:HH2	1:A:346:GLU:HG3	1.85	0.41
1:B:368:LEU:HD22	1:B:373:PHE:HE2	1.85	0.41
1:A:293:ILE:O	1:A:297:LEU:HD23	2.20	0.41
1:A:636:LEU:CD1	1:A:670:THR:HG21	2.51	0.41
1:B:933:MET:HA	1:B:934:PRO:HD3	1.89	0.41
1:B:625:ARG:HB2	1:B:678:MET:HE1	2.02	0.41
1:B:639:GLN:N	1:B:639:GLN:OE1	2.54	0.41
1:A:709:ILE:HA	1:A:709:ILE:HD13	1.77	0.41
1:B:794:TYR:HB3	1:B:821:HIS:NE2	2.35	0.41
1:B:608:ILE:HA	1:B:608:ILE:HD13	1.89	0.41
1:A:573:HIS:CD2	1:A:573:HIS:C	2.94	0.41
1:B:653:PRO:HB3	1:B:661:TYR:CE1	2.55	0.41
1:A:299:THR:HA	1:A:302:TYR:CZ	2.48	0.41
1:B:804:GLY:O	1:B:805:ASP:CB	2.69	0.41
1:A:641:MET:HE3	1:A:641:MET:HB3	1.92	0.41
1:B:400:GLN:HG2	1:B:881:LEU:HD22	2.02	0.41
1:A:727:LEU:N	1:A:727:LEU:HD23	2.35	0.41
1:B:333:THR:O	1:B:337:LYS:HG3	2.21	0.41
1:B:342:LYS:HG3	1:B:346:GLU:CD	2.41	0.41
1:B:302:TYR:CE2	1:B:303:ARG:NE	2.86	0.41
1:B:302:TYR:HD1	1:B:330:LYS:HB2	1.86	0.41
1:A:298:HIS:HB3	1:A:302:TYR:CZ	2.51	0.41
1:A:828:LEU:O	1:A:830:ARG:NH1	2.54	0.41
1:B:830:ARG:NH2	1:B:903:LYS:HZ2	2.19	0.41
1:B:751:THR:HG22	1:B:754:GLU:HG3	2.02	0.41
1:B:307:THR:O	1:B:308:TYR:HD2	2.04	0.41
1:A:585:LYS:HA	1:A:585:LYS:HD2	1.78	0.41
1:A:333:THR:HG21	1:A:364:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1949:093:NAU	2:A:1949:093:CL	2.91	0.41
1:B:806:ARG:HH22	1:B:823:ASP:H	1.69	0.41
1:B:923:SER:O	1:B:927:VAL:HG22	2.21	0.41
1:A:580:LEU:HD23	1:A:580:LEU:O	2.21	0.40
1:B:678:MET:C	1:B:699:HIS:NE2	2.60	0.40
1:A:676:ALA:O	1:A:677:LEU:C	2.59	0.40
1:A:841:LEU:HD23	1:A:845:MET:HE2	2.02	0.40
1:A:303:ARG:O	1:A:304:TYR:HD2	2.03	0.40
1:A:400:GLN:OE1	1:A:711:GLN:OE1	2.38	0.40
1:B:709:ILE:HA	1:B:709:ILE:HD13	1.93	0.40
1:B:850:GLY:O	1:B:854:SER:HB3	2.21	0.40
1:A:810:ASN:HB3	1:A:811:LEU:HD23	2.03	0.40
1:B:610:GLU:HG3	1:B:644:VAL:H	1.87	0.40
1:A:824:PHE:HB3	1:A:827:ILE:HD11	2.03	0.40
1:A:888:ALA:O	1:A:889:THR:CG2	2.70	0.40
1:B:604:GLN:HE21	1:B:653:PRO:HG2	1.86	0.40
1:A:379:ARG:O	1:A:383:VAL:HG23	2.21	0.40
1:A:314:GLU:HG3	1:A:314:GLU:H	1.76	0.40
1:B:318:VAL:O	1:B:319:TRP:C	2.58	0.40
1:A:305:PRO:HA	1:A:306:PRO:HD3	1.91	0.40
1:B:718:LYS:O	1:B:722:ARG:HG3	2.21	0.40
1:A:885:MET:O	1:A:888:ALA:HB2	2.21	0.40
1:A:674:LYS:HD3	1:A:674:LYS:H	1.86	0.40
1:B:603:LYS:HE3	1:B:652:ILE:HG12	2.04	0.40
1:B:843:LYS:HA	1:B:932:VAL:CG1	2.51	0.40
1:A:925:LEU:O	1:A:929:ILE:HG13	2.21	0.40
1:B:557:ILE:HD11	1:B:736:ALA:O	2.21	0.40

All (2) 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:A:661:TYR:OH	1:A:782:GLU:OE1[6_555]	2.07	0.13
1:B:391:ASP:OD2	1:B:724:ASN:ND2[8_565]	2.18	0.02

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	539/696 (77%)	505 (94%)	30 (6%)	4 (1%)	26	72
1	B	540/696 (78%)	517 (96%)	20 (4%)	3 (1%)	30	75
All	All	1079/1392 (78%)	1022 (95%)	50 (5%)	7 (1%)	30	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	SER
1	A	305	PRO
1	B	408	GLU
1	A	304	TYR
1	A	591	ASN
1	B	889	THR
1	A	679	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	490/612 (80%)	398 (81%)	92 (19%)	2	11
1	B	490/612 (80%)	395 (81%)	95 (19%)	2	10
All	All	980/1224 (80%)	793 (81%)	187 (19%)	2	10

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	LEU
1	A	302	TYR
1	A	316	ASP
1	A	317	LEU
1	A	333	THR
1	A	335	PHE
1	A	339	ILE
1	A	341	TRP
1	A	343	LEU
1	A	351	LEU
1	A	354	LEU
1	A	357	TRP
1	A	361	ASP
1	A	363	GLU
1	A	370	SER
1	A	373	PHE
1	A	378	VAL
1	A	391	ASP
1	A	400	GLN
1	A	409	ASP
1	A	415	HIS
1	A	416	LEU
1	A	417	HIS
1	A	419	CYS
1	A	532	ASN
1	A	533	LEU
1	A	549	ASN
1	A	556	SER
1	A	569	ASP
1	A	573	HIS
1	A	575	MET
1	A	578	MET
1	A	581	LYS
1	A	602	ARG
1	A	611	LEU
1	A	612	VAL
1	A	614	LEU
1	A	617	LEU
1	A	625	ARG
1	A	629	THR
1	A	632	PHE
1	A	634	LYS
1	A	639	GLN

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Mol	Chain	Res	Type
1	A	641	MET
1	A	645	ASN
1	A	649	PHE
1	A	654	PHE
1	A	656	LEU
1	A	657	ASP
1	A	663	THR
1	A	668	MET
1	A	669	ARG
1	A	670	THR
1	A	674	LYS
1	A	677	LEU
1	A	678	MET
1	A	682	LEU
1	A	683	THR
1	A	688	ILE
1	A	702	ASP
1	A	705	GLN
1	A	706	ASP
1	A	710	LEU
1	A	722	ARG
1	A	723	GLU
1	A	747	VAL
1	A	748	ASP
1	A	750	CYS
1	A	751	THR
1	A	759	GLU
1	A	765	PHE
1	A	773	ASP
1	A	782	GLU
1	A	790	SER
1	A	808	LEU
1	A	811	LEU
1	A	813	LEU
1	A	835	MET
1	A	839	MET
1	A	842	SER
1	A	860	PHE
1	A	878	MET
1	A	889	THR
1	A	895	LEU
1	A	896	GLU

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Mol	Chain	Res	Type
1	A	898	ASP
1	A	913	THR
1	A	920	HIS
1	A	927	VAL
1	A	930	THR
1	A	940	ILE
1	A	944	THR
1	B	293	ILE
1	B	295	ASP
1	B	297	LEU
1	B	298	HIS
1	B	300	ILE
1	B	302	TYR
1	B	308	TYR
1	B	310	LEU
1	B	313	GLU
1	B	316	ASP
1	B	317	LEU
1	B	318	VAL
1	B	321	PHE
1	B	322	ARG
1	B	328	HIS
1	B	329	LYS
1	B	332	LEU
1	B	335	PHE
1	B	336	LEU
1	B	344	GLU
1	B	346	GLU
1	B	366	LEU
1	B	367	GLU
1	B	398	LEU
1	B	399	LEU
1	B	419	CYS
1	B	543	THR
1	B	544	ASN
1	B	546	THR
1	B	547	LEU
1	B	549	ASN
1	B	556	SER
1	B	569	ASP
1	B	570	GLU
1	B	573	HIS

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Mol	Chain	Res	Type
1	B	579	VAL
1	B	580	LEU
1	B	591	ASN
1	B	599	TYR
1	B	611	LEU
1	B	614	LEU
1	B	624	ASN
1	B	631	LYS
1	B	634	LYS
1	B	635	LEU
1	B	639	GLN
1	B	640	ASP
1	B	641	MET
1	B	643	LYS
1	B	644	VAL
1	B	645	ASN
1	B	654	PHE
1	B	656	LEU
1	B	663	THR
1	B	670	THR
1	B	677	LEU
1	B	678	MET
1	B	691	HIS
1	B	704	ARG
1	B	706	ASP
1	B	708	LEU
1	B	714	THR
1	B	715	LEU
1	B	725	LEU
1	B	741	HIS
1	B	758	ARG
1	B	765	PHE
1	B	773	ASP
1	B	779	ILE
1	B	786	THR
1	B	788	ILE
1	B	806	ARG
1	B	811	LEU
1	B	812	LEU
1	B	813	LEU
1	B	814	THR
1	B	819	LEU

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Mol	Chain	Res	Type
1	B	822	ILE
1	B	827	ILE
1	B	835	MET
1	B	839	MET
1	B	852	ILE
1	B	854	SER
1	B	855	GLU
1	B	859	GLU
1	B	860	PHE
1	B	866	THR
1	B	876	ASN
1	B	877	VAL
1	B	879	LEU
1	B	889	THR
1	B	913	THR
1	B	927	VAL
1	B	945	GLN
1	B	948	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	375	HIS
1	A	403	GLN
1	A	412	HIS
1	A	549	ASN
1	A	573	HIS
1	A	639	GLN
1	A	645	ASN
1	A	691	HIS
1	A	711	GLN
1	A	741	HIS
1	A	769	HIS
1	A	770	HIS
1	A	807	HIS
1	A	810	ASN
1	A	870	HIS
1	A	922	GLN
1	B	403	GLN
1	B	549	ASN
1	B	568	GLN

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Mol	Chain	Res	Type
1	B	573	HIS
1	B	633	GLN
1	B	711	GLN
1	B	724	ASN
1	B	807	HIS
1	B	870	HIS
1	B	876	ASN
1	B	907	ASN
1	B	939	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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$
2	093	A	1949	-	21,25,25	3.73	13 (61%)	24,36,36	2.78	11 (45%)
2	093	B	1950	-	21,25,25	3.97	14 (66%)	24,36,36	3.05	11 (45%)

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
2	093	A	1949	-	-	0/17/19/19	0/2/2/2
2	093	B	1950	-	-	2/17/19/19	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1950	093	CAB-CAF	-2.38	1.36	1.40
2	A	1949	093	CAB-CAF	-2.33	1.36	1.40
2	A	1949	093	CAC-CAB	2.33	1.44	1.39
2	B	1950	093	CAB-CL	2.37	1.79	1.73
2	A	1949	093	CAF-SAN	2.69	1.81	1.77
2	B	1950	093	CAC-CAB	2.72	1.44	1.39
2	A	1949	093	CAT-CAS	2.86	1.53	1.49
2	A	1949	093	OAM-SAN	2.95	1.46	1.43
2	B	1950	093	CAF-SAN	3.30	1.82	1.77
2	A	1949	093	CAH-CAI	3.37	1.51	1.48
2	B	1950	093	OAM-SAN	3.54	1.47	1.43
2	B	1950	093	CAT-CAS	3.66	1.54	1.49
2	B	1950	093	OAO-SAN	3.70	1.47	1.43
2	A	1949	093	CAS-NAR	3.87	1.46	1.37
2	A	1949	093	OAO-SAN	3.97	1.47	1.43
2	B	1950	093	CAS-NAR	4.09	1.47	1.37
2	B	1950	093	CAQ-NAR	4.27	1.45	1.33
2	A	1949	093	CAQ-NAR	4.34	1.45	1.33
2	B	1950	093	CAH-CAI	4.51	1.52	1.48
2	A	1949	093	CAD-CAC	4.52	1.46	1.38
2	B	1950	093	CAD-CAC	5.05	1.47	1.38
2	A	1949	093	CAG-CAF	5.85	1.48	1.39
2	B	1950	093	CAG-CAF	6.57	1.49	1.39
2	A	1949	093	CAI-CAJ	7.28	1.58	1.37
2	B	1950	093	CAI-CAJ	7.67	1.59	1.37
2	B	1950	093	SAN-NAU	8.51	1.72	1.61
2	A	1949	093	SAN-NAU	8.94	1.73	1.61

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1949	093	OAO-SAN-OAM	-8.14	108.74	119.54
2	B	1950	093	OAO-SAN-OAM	-6.51	110.90	119.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1950	093	CAB-CAF-SAN	-6.29	119.44	123.30
2	B	1950	093	CAF-CAB-CL	-5.28	117.70	121.54
2	A	1949	093	CAB-CAF-SAN	-3.74	121.01	123.30
2	A	1949	093	CAF-CAB-CL	-3.73	118.83	121.54
2	B	1950	093	OAL-CAS-NAR	-3.49	116.88	123.68
2	A	1949	093	CAV-NAU-SAN	-2.38	111.52	120.43
2	B	1950	093	CAV-NAU-SAN	-2.27	111.92	120.43
2	A	1949	093	OAM-SAN-CAF	-2.12	104.14	107.63
2	B	1950	093	CAC-CAB-CL	2.03	122.59	118.39
2	A	1949	093	OAO-SAN-CAF	2.08	111.06	107.63
2	B	1950	093	CAD-CAH-CAG	2.08	120.93	118.17
2	A	1949	093	OAO-SAN-NAU	2.53	111.10	107.03
2	B	1950	093	OAO-SAN-NAU	2.71	111.39	107.03
2	B	1950	093	CAQ-NAR-CAS	2.72	123.33	115.92
2	A	1949	093	CAD-CAH-CAG	2.93	122.06	118.17
2	A	1949	093	OAM-SAN-NAU	3.00	111.85	107.03
2	A	1949	093	CAT-CAS-NAR	3.45	120.35	114.91
2	B	1950	093	CAW-CAV-NAU	3.62	117.10	110.34
2	A	1949	093	CAW-CAV-NAU	4.57	118.88	110.34
2	B	1950	093	CAT-CAS-NAR	6.34	124.91	114.91

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1950	093	OAL-CAS-NAR-CAQ
2	B	1950	093	CAT-CAS-NAR-CAQ

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1949	093	8	0
2	B	1950	093	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	545/696 (78%)	-0.26	3 (0%) 90 85	32, 55, 105, 116	0
1	B	546/696 (78%)	-0.15	5 (0%) 85 78	43, 65, 116, 123	0
All	All	1091/1392 (78%)	-0.20	8 (0%) 89 82	32, 61, 107, 123	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	TRP	3.1
1	A	302	TYR	2.7
1	B	636	LEU	2.5
1	B	423	GLU	2.2
1	A	322	ARG	2.2
1	B	347	VAL	2.2
1	A	298	HIS	2.1
1	B	377	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(\AA^2)	Q<0.9
2	093	A	1949	24/24	0.89	0.31	1.79	87,97,104,107	0
2	093	B	1950	24/24	0.91	0.35	1.08	101,108,117,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.