



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:40 PM UTC

PDB ID : 5L5G / pdb_00005l5g
Title : Plexin A2 full extracellular region, domains 1 to 8 modeled, data to 10 angstrom
Authors : Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.
Deposited on : 2016-05-28
Resolution : 10.00 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
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

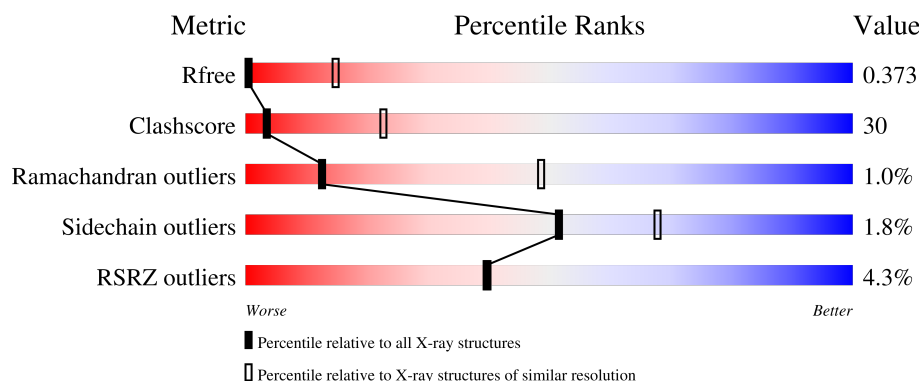
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 10.00 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	1168 (11.50-4.00)
Clashscore	190562	1002 (15.00-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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	1212	4% 50% 22% •• 25%
1	B	1212	2% 45% 20% • 33%
1	C	1212	4% 52% 26% • 18%
1	D	1212	3% 52% 27% •• 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28787 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 Plexin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	906	Total	C	N	O	S	0	0	0
			7060	4461	1214	1333	52			
1	B	809	Total	C	N	O	S	0	0	0
			6337	4004	1092	1195	46			
1	C	993	Total	C	N	O	S	0	0	0
			7695	4856	1321	1462	56			
1	D	993	Total	C	N	O	S	0	0	0
			7695	4856	1321	1462	56			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLU	-	expression tag	UNP P70207
A	1232	GLY	-	expression tag	UNP P70207
A	1233	GLY	-	expression tag	UNP P70207
A	1234	SER	-	expression tag	UNP P70207
A	1235	ARG	-	expression tag	UNP P70207
A	1236	THR	-	expression tag	UNP P70207
A	1237	LYS	-	expression tag	UNP P70207
A	1238	HIS	-	expression tag	UNP P70207
A	1239	HIS	-	expression tag	UNP P70207
A	1240	HIS	-	expression tag	UNP P70207
A	1241	HIS	-	expression tag	UNP P70207
A	1242	HIS	-	expression tag	UNP P70207
A	1243	HIS	-	expression tag	UNP P70207
B	32	GLU	-	expression tag	UNP P70207
B	1232	GLY	-	expression tag	UNP P70207
B	1233	GLY	-	expression tag	UNP P70207
B	1234	SER	-	expression tag	UNP P70207
B	1235	ARG	-	expression tag	UNP P70207
B	1236	THR	-	expression tag	UNP P70207
B	1237	LYS	-	expression tag	UNP P70207
B	1238	HIS	-	expression tag	UNP P70207

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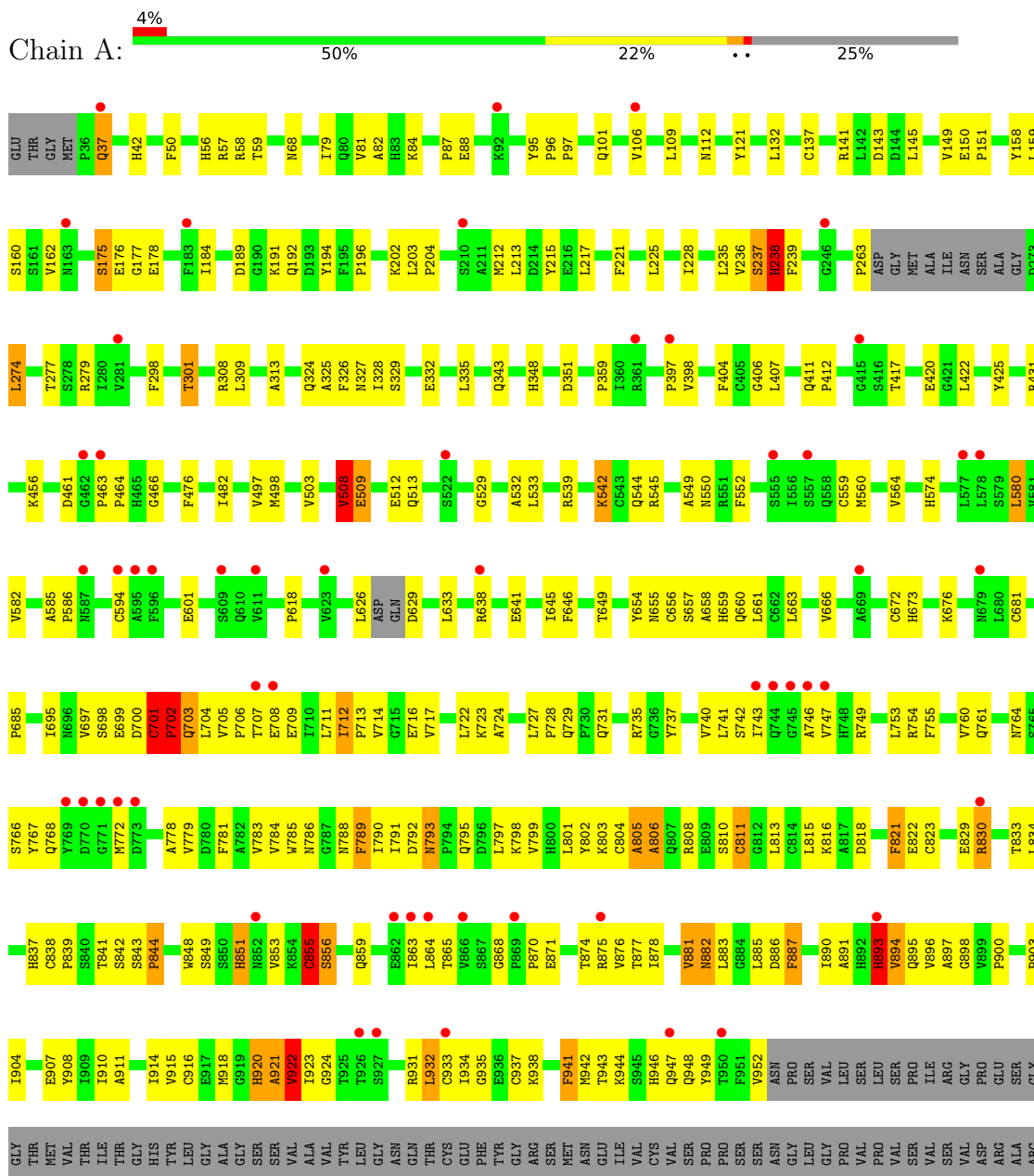
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	HIS	-	expression tag	UNP P70207
B	1240	HIS	-	expression tag	UNP P70207
B	1241	HIS	-	expression tag	UNP P70207
B	1242	HIS	-	expression tag	UNP P70207
B	1243	HIS	-	expression tag	UNP P70207
C	32	GLU	-	expression tag	UNP P70207
C	1232	GLY	-	expression tag	UNP P70207
C	1233	GLY	-	expression tag	UNP P70207
C	1234	SER	-	expression tag	UNP P70207
C	1235	ARG	-	expression tag	UNP P70207
C	1236	THR	-	expression tag	UNP P70207
C	1237	LYS	-	expression tag	UNP P70207
C	1238	HIS	-	expression tag	UNP P70207
C	1239	HIS	-	expression tag	UNP P70207
C	1240	HIS	-	expression tag	UNP P70207
C	1241	HIS	-	expression tag	UNP P70207
C	1242	HIS	-	expression tag	UNP P70207
C	1243	HIS	-	expression tag	UNP P70207
D	32	GLU	-	expression tag	UNP P70207
D	1232	GLY	-	expression tag	UNP P70207
D	1233	GLY	-	expression tag	UNP P70207
D	1234	SER	-	expression tag	UNP P70207
D	1235	ARG	-	expression tag	UNP P70207
D	1236	THR	-	expression tag	UNP P70207
D	1237	LYS	-	expression tag	UNP P70207
D	1238	HIS	-	expression tag	UNP P70207
D	1239	HIS	-	expression tag	UNP P70207
D	1240	HIS	-	expression tag	UNP P70207
D	1241	HIS	-	expression tag	UNP P70207
D	1242	HIS	-	expression tag	UNP P70207
D	1243	HIS	-	expression tag	UNP P70207

3 Residue-property plots

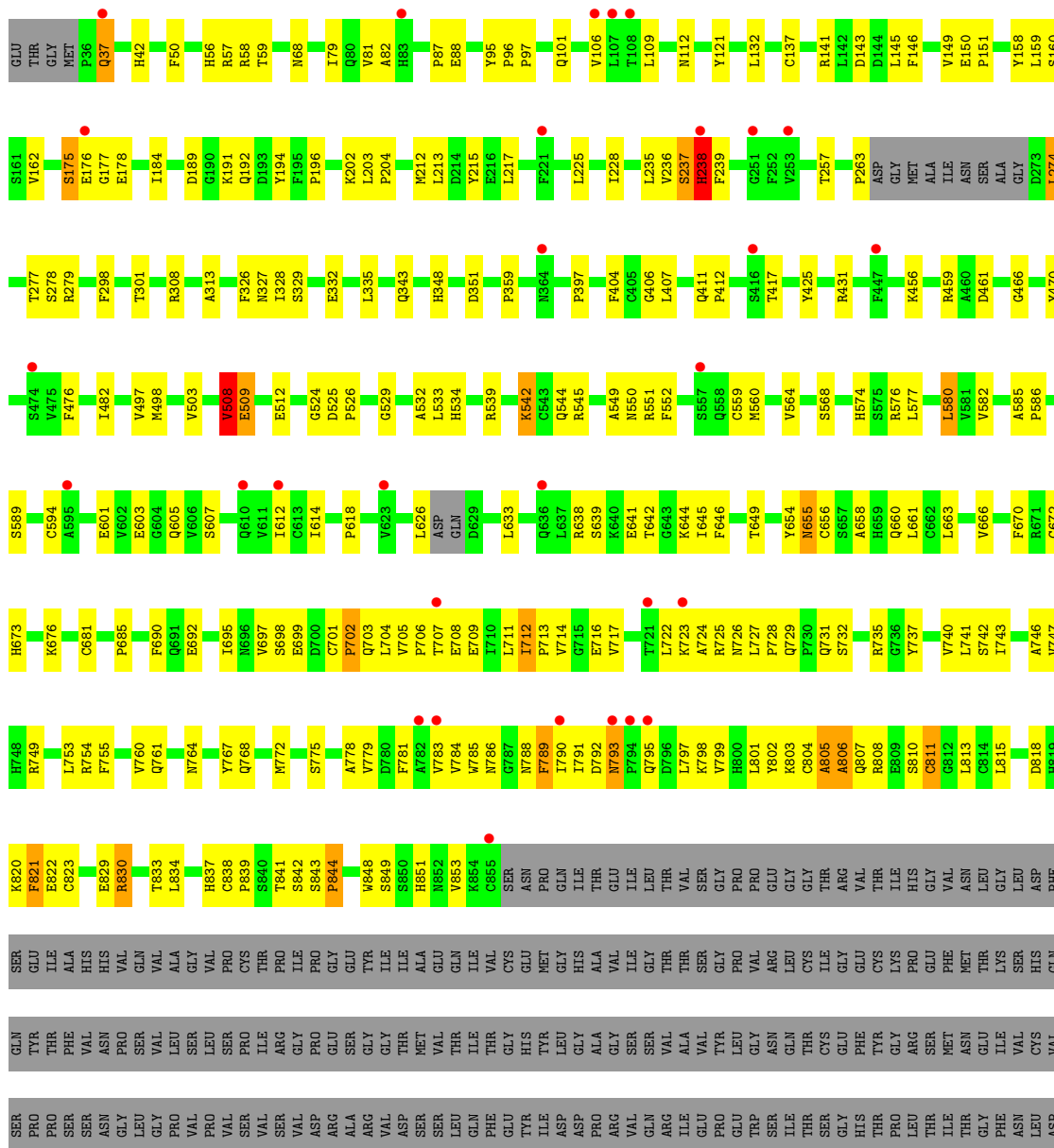
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Plexin-A2

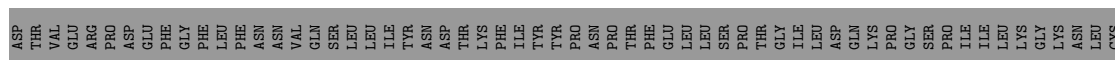


[illegible]

- Molecule 1: Plexin-A2



- Molecule 1: Plexin-A2



Chain D:



ASP
GLY
GLY
SER
ARG
THR
LYS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	238.40 Å 238.40 Å 642.18 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.05 – 10.00 63.05 – 10.00	Depositor EDS
% Data completeness (in resolution range)	92.5 (63.05-10.00) 92.6 (63.05-10.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.335 , 0.370 0.334 , 0.373	Depositor DCC
R_{free} test set	529 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 73.4	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	28787	wwPDB-VP
Average B, all atoms (Å ²)	236.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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 ⓘ

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	1.01	12/7230 (0.2%)	1.16	43/9821 (0.4%)
1	B	1.02	9/6488 (0.1%)	1.32	25/8804 (0.3%)
1	C	0.90	15/7878 (0.2%)	1.24	50/10705 (0.5%)
1	D	0.97	15/7879 (0.2%)	1.33	60/10708 (0.6%)
All	All	0.97	51/29475 (0.2%)	1.26	178/40038 (0.4%)

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	2
1	B	0	1
1	C	0	4
1	D	0	4
All	All	0	11

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	702	PRO	C-N	49.52	1.94	1.33
1	A	702	PRO	C-N	39.90	1.89	1.33
1	A	508	VAL	C-N	-38.57	0.78	1.33
1	D	655	ASN	C-N	-28.75	0.96	1.34
1	B	655	ASN	C-N	28.02	1.71	1.34
1	D	508	VAL	C-N	-25.36	0.98	1.33
1	B	508	VAL	C-N	-24.51	0.99	1.33
1	C	508	VAL	C-N	-21.04	1.07	1.33
1	C	701	CYS	C-N	16.23	1.60	1.34
1	D	952	VAL	C-N	15.86	1.66	1.33
1	D	559	CYS	C-N	11.88	1.48	1.33
1	A	803	LYS	C-N	-11.32	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	803	LYS	C-N	-9.75	1.20	1.33
1	D	803	LYS	C-N	9.18	1.46	1.33
1	D	988	TYR	CB-CG	-7.80	1.34	1.51
1	C	988	TYR	CB-CG	-7.79	1.34	1.51
1	D	988	TYR	CA-CB	7.39	1.65	1.53
1	C	988	TYR	CA-CB	7.28	1.65	1.53
1	A	701	CYS	C-N	-5.95	1.20	1.33
1	C	952	VAL	C-N	-5.88	1.21	1.33
1	C	988	TYR	CA-C	5.46	1.58	1.52
1	D	988	TYR	CA-C	5.44	1.58	1.52
1	C	712	ILE	CA-CB	-5.43	1.50	1.54
1	B	712	ILE	CA-CB	-5.42	1.50	1.54
1	C	988	TYR	N-CA	-5.41	1.39	1.46
1	A	712	ILE	CA-CB	-5.41	1.50	1.54
1	D	988	TYR	N-CA	-5.41	1.39	1.46
1	C	37	GLN	CD-OE1	5.40	1.33	1.23
1	D	37	GLN	CD-OE1	5.36	1.33	1.23
1	A	37	GLN	CD-OE1	5.35	1.33	1.23
1	B	37	GLN	CD-OE1	5.35	1.33	1.23
1	C	238	HIS	ND1-CE1	5.29	1.37	1.32
1	D	712	ILE	CA-CB	-5.29	1.50	1.54
1	A	42	HIS	ND1-CE1	5.25	1.37	1.32
1	B	238	HIS	ND1-CE1	5.24	1.37	1.32
1	B	42	HIS	ND1-CE1	5.24	1.37	1.32
1	D	42	HIS	ND1-CE1	5.23	1.37	1.32
1	D	238	HIS	ND1-CE1	5.23	1.37	1.32
1	C	42	HIS	ND1-CE1	5.22	1.37	1.32
1	A	238	HIS	ND1-CE1	5.20	1.37	1.32
1	A	844	PRO	C-N	5.19	1.40	1.33
1	B	844	PRO	C-N	5.14	1.40	1.33
1	C	101	GLN	CD-OE1	5.13	1.33	1.23
1	B	101	GLN	CD-OE1	5.10	1.33	1.23
1	D	101	GLN	CD-OE1	5.10	1.33	1.23
1	D	844	PRO	C-N	5.09	1.40	1.33
1	A	855	CYS	C-N	5.09	1.40	1.33
1	A	101	GLN	CD-OE1	5.09	1.33	1.23
1	C	844	PRO	C-N	5.08	1.40	1.33
1	A	513	GLN	CD-OE1	5.05	1.33	1.23
1	C	513	GLN	CD-OE1	5.03	1.33	1.23

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	PRO	O-C-N	-65.13	51.99	122.98
1	B	508	VAL	O-C-N	-42.43	69.54	122.57
1	C	803	LYS	O-C-N	-36.79	72.31	121.97
1	D	559	CYS	O-C-N	-36.52	74.01	122.59
1	D	508	VAL	O-C-N	21.65	144.24	121.94
1	D	508	VAL	CA-C-N	-21.35	91.97	122.93
1	D	508	VAL	C-N-CA	-21.35	91.97	122.93
1	D	988	TYR	CA-CB-CG	-20.75	76.55	113.90
1	C	988	TYR	CA-CB-CG	-20.72	76.60	113.90
1	A	701	CYS	CA-C-N	-19.94	94.92	119.84
1	A	701	CYS	C-N-CA	-19.94	94.92	119.84
1	D	952	VAL	O-C-N	-19.03	98.79	122.57
1	A	508	VAL	O-C-N	-15.78	105.93	121.87
1	C	844	PRO	N-CA-C	15.14	133.52	113.98
1	B	844	PRO	N-CA-C	15.13	133.50	113.98
1	A	844	PRO	N-CA-C	15.13	133.50	113.98
1	D	844	PRO	N-CA-C	15.13	133.50	113.98
1	B	702	PRO	CA-C-N	14.14	147.50	121.62
1	B	702	PRO	C-N-CA	14.14	147.50	121.62
1	C	988	TYR	CB-CG-CD1	-13.59	100.41	120.80
1	D	988	TYR	CB-CG-CD1	-13.51	100.53	120.80
1	A	702	PRO	O-C-N	-13.11	104.94	122.64
1	D	559	CYS	CA-C-N	13.11	145.06	121.85
1	D	559	CYS	C-N-CA	13.11	145.06	121.85
1	D	701	CYS	O-C-N	12.80	151.37	121.93
1	C	988	TYR	CD1-CG-CD2	11.79	135.78	118.10
1	D	988	TYR	CD1-CG-CD2	11.73	135.69	118.10
1	A	508	VAL	CA-C-N	11.53	142.21	122.37
1	A	508	VAL	C-N-CA	11.53	142.21	122.37
1	C	988	TYR	CG-CD2-CE2	-11.11	104.53	121.20
1	D	988	TYR	CG-CD2-CE2	-11.10	104.56	121.20
1	D	803	LYS	CA-C-N	-10.98	100.58	121.54
1	D	803	LYS	C-N-CA	-10.98	100.58	121.54
1	C	941	PHE	CA-CB-CG	-10.43	103.37	113.80
1	A	941	PHE	CA-CB-CG	-10.38	103.42	113.80
1	D	941	PHE	CA-CB-CG	-10.38	103.42	113.80
1	A	855	CYS	O-C-N	-9.21	109.73	122.81
1	D	755	PHE	CA-CB-CG	-8.69	105.11	113.80
1	A	755	PHE	CA-CB-CG	-8.64	105.16	113.80
1	B	755	PHE	CA-CB-CG	-8.64	105.16	113.80
1	C	755	PHE	CA-CB-CG	-8.58	105.22	113.80
1	B	508	VAL	CA-C-N	8.52	137.82	121.54
1	B	508	VAL	C-N-CA	8.52	137.82	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1012	SER	N-CA-C	-7.91	103.52	113.01
1	A	855	CYS	CA-C-N	-7.86	109.61	122.81
1	A	855	CYS	C-N-CA	-7.86	109.61	122.81
1	C	1012	SER	N-CA-C	-7.83	103.62	113.01
1	C	841	THR	N-CA-C	-7.78	102.88	111.36
1	B	841	THR	N-CA-C	-7.78	102.88	111.36
1	D	841	THR	N-CA-C	-7.77	102.89	111.36
1	D	893	HIS	CA-CB-CG	7.76	121.56	113.80
1	A	841	THR	N-CA-C	-7.76	102.90	111.36
1	C	803	LYS	CA-C-N	-7.73	106.78	121.54
1	C	803	LYS	C-N-CA	-7.73	106.78	121.54
1	A	893	HIS	CA-CB-CG	7.72	121.52	113.80
1	A	881	VAL	N-CA-C	7.70	118.61	111.45
1	C	893	HIS	CA-CB-CG	7.69	121.49	113.80
1	D	881	VAL	N-CA-C	7.68	118.60	111.45
1	C	881	VAL	N-CA-C	7.67	118.59	111.45
1	C	655	ASN	CA-C-N	-7.52	107.17	121.54
1	C	655	ASN	C-N-CA	-7.52	107.17	121.54
1	D	952	VAL	CA-C-N	7.50	140.10	121.80
1	D	952	VAL	C-N-CA	7.50	140.10	121.80
1	D	990	GLY	CA-C-N	7.29	135.47	121.54
1	D	990	GLY	C-N-CA	7.29	135.47	121.54
1	C	990	GLY	CA-C-N	7.28	135.45	121.54
1	C	990	GLY	C-N-CA	7.28	135.45	121.54
1	D	701	CYS	CA-C-N	-7.19	86.63	122.60
1	D	701	CYS	C-N-CA	-7.19	86.63	122.60
1	B	821	PHE	CA-CB-CG	-7.05	106.75	113.80
1	D	821	PHE	CA-CB-CG	-7.05	106.75	113.80
1	C	821	PHE	CA-CB-CG	-7.00	106.80	113.80
1	A	821	PHE	CA-CB-CG	-6.97	106.83	113.80
1	C	1025	ASP	CB-CA-C	-6.95	108.57	116.63
1	D	1025	ASP	CB-CA-C	-6.92	108.60	116.63
1	D	701	CYS	C-N-CD	6.64	152.21	125.00
1	C	42	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	D	42	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	A	42	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	D	922	VAL	CA-C-N	6.58	131.98	123.03
1	D	922	VAL	C-N-CA	6.58	131.98	123.03
1	C	922	VAL	CA-C-N	6.58	131.97	123.03
1	C	922	VAL	C-N-CA	6.58	131.97	123.03
1	A	238	HIS	CB-CG-CD2	-6.56	122.68	131.20
1	B	238	HIS	CB-CG-CD2	-6.55	122.69	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	238	HIS	CB-CG-CD2	-6.55	122.69	131.20
1	C	844	PRO	CA-C-O	-6.54	109.01	118.89
1	A	922	VAL	CA-C-N	6.53	131.91	123.03
1	A	922	VAL	C-N-CA	6.53	131.91	123.03
1	D	844	PRO	CA-C-O	-6.52	109.04	118.89
1	B	42	HIS	CB-CG-CD2	-6.52	122.73	131.20
1	A	844	PRO	CA-C-O	-6.51	109.06	118.89
1	C	238	HIS	CB-CG-CD2	-6.50	122.74	131.20
1	B	844	PRO	CA-C-O	-6.48	109.10	118.89
1	C	921	ALA	N-CA-C	6.45	120.99	113.18
1	A	921	ALA	N-CA-C	6.43	120.96	113.18
1	D	921	ALA	N-CA-C	6.42	120.95	113.18
1	D	806	ALA	N-CA-C	-6.28	104.32	112.23
1	C	806	ALA	N-CA-C	-6.28	104.32	112.23
1	A	806	ALA	N-CA-C	-6.26	104.34	112.23
1	B	806	ALA	N-CA-C	-6.23	104.38	112.23
1	D	991	ASN	CA-C-N	6.06	129.43	120.95
1	D	991	ASN	C-N-CA	6.06	129.43	120.95
1	C	991	ASN	CA-C-N	6.04	129.40	120.95
1	C	991	ASN	C-N-CA	6.04	129.40	120.95
1	C	701	CYS	O-C-N	5.98	126.85	121.35
1	A	887	PHE	CA-CB-CG	-5.87	107.93	113.80
1	B	348	HIS	CA-C-N	5.85	123.93	119.66
1	B	348	HIS	C-N-CA	5.85	123.93	119.66
1	C	887	PHE	CA-CB-CG	-5.84	107.95	113.80
1	D	887	PHE	CA-CB-CG	-5.76	108.04	113.80
1	A	348	HIS	CA-C-N	5.71	123.83	119.66
1	A	348	HIS	C-N-CA	5.71	123.83	119.66
1	C	42	HIS	CB-CG-ND1	5.69	131.24	122.70
1	C	988	TYR	CB-CA-C	5.69	119.24	110.14
1	D	348	HIS	CA-C-N	5.69	123.81	119.66
1	D	348	HIS	C-N-CA	5.69	123.81	119.66
1	A	856	SER	CA-C-N	5.69	128.56	123.10
1	A	856	SER	C-N-CA	5.69	128.56	123.10
1	A	238	HIS	CB-CG-ND1	5.68	131.22	122.70
1	D	42	HIS	CB-CG-ND1	5.68	131.22	122.70
1	D	238	HIS	CB-CG-ND1	5.67	131.21	122.70
1	C	348	HIS	CA-C-N	5.67	123.80	119.66
1	C	348	HIS	C-N-CA	5.67	123.80	119.66
1	D	988	TYR	CB-CA-C	5.64	119.16	110.14
1	B	238	HIS	CB-CG-ND1	5.63	131.15	122.70
1	B	42	HIS	CB-CG-ND1	5.63	131.14	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	238	HIS	CB-CG-ND1	5.62	131.13	122.70
1	A	42	HIS	CB-CG-ND1	5.62	131.12	122.70
1	D	894	VAL	CB-CA-C	-5.55	103.46	111.34
1	A	894	VAL	CB-CA-C	-5.54	103.48	111.34
1	C	894	VAL	CB-CA-C	-5.52	103.50	111.34
1	B	788	ASN	CA-CB-CG	-5.51	107.09	112.60
1	D	788	ASN	CA-CB-CG	-5.50	107.10	112.60
1	C	788	ASN	CA-CB-CG	-5.47	107.13	112.60
1	D	991	ASN	CA-CB-CG	-5.45	107.15	112.60
1	A	788	ASN	CA-CB-CG	-5.44	107.16	112.60
1	C	991	ASN	CA-CB-CG	-5.43	107.17	112.60
1	C	655	ASN	O-C-N	5.34	130.98	122.81
1	D	856	SER	CA-C-N	5.33	128.59	122.83
1	D	856	SER	C-N-CA	5.33	128.59	122.83
1	D	830	ARG	N-CA-C	-5.33	106.08	112.58
1	C	856	SER	CA-C-N	5.32	128.57	122.83
1	C	856	SER	C-N-CA	5.32	128.57	122.83
1	B	830	ARG	N-CA-C	-5.29	106.12	112.58
1	A	882	ASN	CB-CA-C	-5.29	104.53	112.09
1	C	882	ASN	CB-CA-C	-5.29	104.53	112.09
1	D	882	ASN	CB-CA-C	-5.29	104.53	112.09
1	A	830	ARG	N-CA-C	-5.27	106.15	112.58
1	C	417	THR	CA-C-N	5.25	125.15	119.85
1	C	417	THR	C-N-CA	5.25	125.15	119.85
1	C	830	ARG	N-CA-C	-5.24	106.19	112.58
1	A	417	THR	CA-C-N	5.21	125.11	119.85
1	A	417	THR	C-N-CA	5.21	125.11	119.85
1	D	417	THR	CA-C-N	5.20	125.10	119.85
1	D	417	THR	C-N-CA	5.20	125.10	119.85
1	A	702	PRO	CA-C-N	-5.19	111.63	121.54
1	A	702	PRO	C-N-CA	-5.19	111.63	121.54
1	C	1025	ASP	CA-CB-CG	-5.15	107.45	112.60
1	D	920	HIS	CA-C-N	5.13	131.59	121.58
1	D	920	HIS	C-N-CA	5.13	131.59	121.58
1	C	920	HIS	CA-C-N	5.13	131.58	121.58
1	C	920	HIS	C-N-CA	5.13	131.58	121.58
1	A	920	HIS	CA-C-N	5.12	131.56	121.58
1	A	920	HIS	C-N-CA	5.12	131.56	121.58
1	D	1011	SER	N-CA-C	-5.12	101.78	109.15
1	D	1025	ASP	CA-CB-CG	-5.11	107.49	112.60
1	B	417	THR	CA-C-N	5.11	125.01	119.85
1	B	417	THR	C-N-CA	5.11	125.01	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1011	SER	N-CA-C	-5.09	101.82	109.15
1	A	789	PHE	CA-CB-CG	-5.06	108.74	113.80
1	B	789	PHE	CA-CB-CG	-5.05	108.75	113.80
1	B	793	ASN	CA-C-N	5.03	124.20	118.97
1	B	793	ASN	C-N-CA	5.03	124.20	118.97
1	A	793	ASN	CA-C-N	5.03	124.20	118.97
1	A	793	ASN	C-N-CA	5.03	124.20	118.97
1	D	964	GLY	CA-C-N	5.02	124.95	119.78
1	D	964	GLY	C-N-CA	5.02	124.95	119.78

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	701	CYS	Mainchain
1	A	855	CYS	Mainchain
1	B	508	VAL	Mainchain
1	C	508	VAL	Mainchain
1	C	803	LYS	Mainchain
1	C	952	VAL	Mainchain
1	C	988	TYR	Sidechain
1	D	508	VAL	Mainchain
1	D	559	CYS	Mainchain
1	D	803	LYS	Mainchain
1	D	988	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7060	0	6854	441	9
1	B	6337	0	6141	356	8
1	C	7695	0	7466	469	5
1	D	7695	0	7468	499	4
All	All	28787	0	27929	1690	13

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 30.

All (1690) 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:463:PRO:HG2	1:B:612:ILE:CG2	1.25	1.55
1:A:407:LEU:CD2	1:C:944:LYS:HD2	1.03	1.48
1:D:533:LEU:CD1	1:D:642:THR:HG23	1.41	1.48
1:B:655:ASN:C	1:B:656:CYS:N	1.71	1.46
1:A:407:LEU:CD2	1:C:944:LYS:CD	1.93	1.43
1:A:702:PRO:O	1:A:703:GLN:CG	1.65	1.41
1:B:533:LEU:CD2	1:B:646:PHE:CG	2.09	1.36
1:C:551:ARG:NH1	1:C:641:GLU:OE2	1.60	1.34
1:B:663:LEU:HD11	1:B:703:GLN:NE2	1.41	1.33
1:B:549:ALA:O	1:B:586:PRO:CB	1.75	1.32
1:D:533:LEU:CB	1:D:642:THR:HG21	1.59	1.30
1:D:533:LEU:O	1:D:644:LYS:HB2	1.32	1.30
1:A:702:PRO:C	1:A:703:GLN:N	1.89	1.29
1:A:508:VAL:O	1:A:509:GLU:N	1.63	1.28
1:C:663:LEU:HD11	1:C:792:ASP:OD2	1.32	1.27
1:A:407:LEU:HD21	1:C:944:LYS:CD	1.56	1.27
1:B:533:LEU:HD23	1:B:646:PHE:CG	1.67	1.25
1:D:550:ASN:HB2	1:D:586:PRO:CB	1.65	1.25
1:B:775:SER:N	1:B:807:GLN:OE1	1.67	1.25
1:B:550:ASN:ND2	1:B:585:ALA:O	1.70	1.24
1:D:550:ASN:CB	1:D:586:PRO:HB3	1.66	1.24
1:A:422:LEU:CD1	1:B:605:GLN:HG2	1.68	1.23
1:A:463:PRO:CG	1:B:612:ILE:CG2	2.18	1.21
1:A:508:VAL:C	1:A:509:GLU:CA	2.13	1.21
1:C:663:LEU:CD1	1:C:792:ASP:OD2	1.90	1.20
1:D:533:LEU:CD1	1:D:642:THR:CG2	2.21	1.19
1:B:549:ALA:O	1:B:586:PRO:HB3	1.02	1.17
1:D:663:LEU:HD12	1:D:792:ASP:CB	1.73	1.17
1:D:775:SER:CB	1:D:807:GLN:HG3	1.72	1.17
1:B:533:LEU:CD2	1:B:646:PHE:CD1	2.28	1.17
1:C:533:LEU:HB3	1:C:642:THR:HG21	1.24	1.17
1:A:655:ASN:C	1:A:656:CYS:N	2.03	1.16
1:B:778:ALA:HB1	1:B:798:LYS:HD2	1.15	1.14
1:D:533:LEU:HB3	1:D:642:THR:CG2	1.76	1.14
1:A:655:ASN:HB3	1:A:658:ALA:HB2	1.15	1.13
1:D:778:ALA:HB1	1:D:798:LYS:HD2	1.15	1.13
1:B:533:LEU:HD22	1:B:646:PHE:CD1	1.82	1.13
1:B:545:ARG:NH1	1:B:641:GLU:OE2	1.80	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:LEU:CD1	1:B:703:GLN:NE2	2.12	1.13
1:A:810:SER:HB2	1:A:882:ASN:OD1	1.49	1.12
1:C:702:PRO:HB3	1:C:728:PRO:HD3	1.18	1.11
1:B:692:GLU:CD	1:D:141:ARG:HH22	1.57	1.11
1:C:932:LEU:HB3	1:C:943:THR:HG22	1.33	1.11
1:D:534:HIS:HA	1:D:644:LYS:HG3	1.32	1.11
1:D:932:LEU:HB3	1:D:943:THR:HG22	1.32	1.11
1:A:932:LEU:HB3	1:A:943:THR:HG22	1.33	1.10
1:D:533:LEU:HD12	1:D:642:THR:HG23	1.16	1.10
1:A:325:ALA:HB2	1:B:577:LEU:HD13	1.12	1.10
1:C:778:ALA:HB1	1:C:798:LYS:HD2	1.15	1.10
1:A:702:PRO:C	1:A:703:GLN:HG3	1.76	1.10
1:A:778:ALA:HB1	1:A:798:LYS:HD2	1.15	1.10
1:A:407:LEU:HD22	1:C:944:LYS:HD2	1.24	1.10
1:A:508:VAL:CA	1:A:509:GLU:N	2.14	1.10
1:C:677:TYR:CD1	1:C:731:GLN:HG3	1.86	1.09
1:A:325:ALA:HB2	1:B:577:LEU:CD1	1.82	1.09
1:D:533:LEU:HB3	1:D:642:THR:HG21	1.20	1.09
1:D:533:LEU:HD13	1:D:642:THR:HG23	1.19	1.09
1:A:532:ALA:HB1	1:A:560:MET:CE	1.83	1.09
1:A:463:PRO:HG2	1:B:612:ILE:HG22	1.10	1.08
1:D:815:LEU:HD23	1:D:853:VAL:HG11	1.33	1.08
1:A:463:PRO:HG2	1:B:612:ILE:CB	1.83	1.07
1:B:803:LYS:C	1:B:804:CYS:N	2.12	1.07
1:A:559:CYS:C	1:A:560:MET:N	2.11	1.07
1:D:958:SER:HA	1:D:1033:LEU:HD22	1.34	1.07
1:B:815:LEU:HD23	1:B:853:VAL:HG11	1.33	1.07
1:C:815:LEU:HD23	1:C:853:VAL:HG11	1.33	1.06
1:D:533:LEU:HD22	1:D:639:SER:CB	1.84	1.06
1:C:958:SER:HA	1:C:1033:LEU:HD22	1.34	1.06
1:D:533:LEU:CD2	1:D:639:SER:CB	2.34	1.06
1:D:775:SER:HB2	1:D:807:GLN:HG3	1.37	1.06
1:A:463:PRO:CG	1:B:612:ILE:HG22	1.83	1.05
1:A:463:PRO:HG2	1:B:612:ILE:HG21	1.33	1.05
1:C:551:ARG:NH1	1:C:641:GLU:CD	2.15	1.05
1:A:325:ALA:CB	1:B:577:LEU:HD13	1.87	1.04
1:D:550:ASN:HD22	1:D:586:PRO:HA	1.14	1.04
1:A:655:ASN:O	1:A:658:ALA:HB3	1.57	1.04
1:A:815:LEU:HD23	1:A:853:VAL:HG11	1.33	1.04
1:B:533:LEU:HD23	1:B:646:PHE:CD2	1.92	1.03
1:A:464:PRO:HB3	1:B:603:GLU:O	1.56	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ALA:HB1	1:A:560:MET:HE3	1.04	1.03
1:A:810:SER:HB2	1:A:882:ASN:CG	1.85	1.02
1:C:663:LEU:HD11	1:C:792:ASP:CG	1.85	1.02
1:C:959:LEU:HG	1:C:974:ILE:HG22	1.41	1.01
1:D:533:LEU:HD22	1:D:639:SER:HB3	1.41	1.01
1:D:661:LEU:HD21	1:D:790:ILE:HD11	1.40	1.00
1:D:959:LEU:HG	1:D:974:ILE:HG22	1.41	1.00
1:B:692:GLU:OE2	1:D:141:ARG:NH2	1.94	1.00
1:A:676:LYS:HE2	1:A:728:PRO:HB3	1.43	1.00
1:B:676:LYS:HE2	1:B:728:PRO:HB3	1.42	1.00
1:D:663:LEU:CD1	1:D:792:ASP:CG	2.35	1.00
1:A:407:LEU:HD23	1:C:944:LYS:HD2	1.43	0.99
1:B:532:ALA:CB	1:B:560:MET:HE3	1.92	0.99
1:B:663:LEU:HD11	1:B:703:GLN:HE22	0.85	0.99
1:C:775:SER:N	1:C:806:ALA:HB3	1.78	0.99
1:D:533:LEU:HD21	1:D:639:SER:HB2	1.42	0.98
1:D:534:HIS:CD2	1:D:644:LYS:HZ3	1.81	0.98
1:C:533:LEU:HB3	1:C:642:THR:CG2	1.93	0.98
1:D:959:LEU:HD13	1:D:1033:LEU:HD23	1.44	0.98
1:B:532:ALA:HB1	1:B:560:MET:HE3	1.01	0.98
1:C:959:LEU:HD13	1:C:1033:LEU:HD23	1.44	0.98
1:D:533:LEU:CD2	1:D:639:SER:HB2	1.91	0.98
1:A:655:ASN:CB	1:A:658:ALA:HB2	1.94	0.98
1:D:533:LEU:CB	1:D:642:THR:CG2	2.37	0.98
1:B:532:ALA:HB1	1:B:560:MET:CE	1.93	0.97
1:A:863:ILE:HD12	1:A:878:ILE:HG12	1.46	0.97
1:D:729:GLN:HG3	1:D:754:ARG:HH12	1.26	0.97
1:A:397:PRO:HB2	1:C:947:GLN:HE22	1.25	0.97
1:A:729:GLN:HG3	1:A:754:ARG:HH12	1.26	0.97
1:C:805:ALA:HB1	1:C:808:ARG:H	1.30	0.97
1:D:663:LEU:CD1	1:D:792:ASP:OD2	2.12	0.97
1:D:863:ILE:HD12	1:D:878:ILE:HG12	1.45	0.97
1:A:407:LEU:HD23	1:C:944:LYS:CE	1.95	0.96
1:A:702:PRO:O	1:A:703:GLN:HG3	0.79	0.96
1:B:729:GLN:HG3	1:B:754:ARG:HH12	1.26	0.96
1:D:805:ALA:HB1	1:D:808:ARG:H	1.30	0.96
1:A:422:LEU:HD11	1:B:605:GLN:HG2	1.46	0.96
1:D:551:ARG:NH1	1:D:641:GLU:OE2	1.99	0.95
1:B:805:ALA:HB1	1:B:808:ARG:H	1.30	0.95
1:A:407:LEU:HD23	1:C:944:LYS:NZ	1.80	0.95
1:D:661:LEU:HD21	1:D:790:ILE:CD1	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:SER:HB2	1:D:83:HIS:CD2	2.01	0.95
1:C:729:GLN:HG3	1:C:754:ARG:HH12	1.26	0.95
1:C:863:ILE:HD12	1:C:878:ILE:HG12	1.45	0.95
1:B:237:SER:HA	1:B:239:PHE:H	1.33	0.94
1:B:735:ARG:HG2	1:B:786:ASN:HA	1.50	0.94
1:C:533:LEU:CB	1:C:642:THR:HG21	1.97	0.94
1:C:735:ARG:HG2	1:C:786:ASN:HA	1.50	0.94
1:D:533:LEU:HB2	1:D:642:THR:HG21	1.45	0.94
1:D:735:ARG:HG2	1:D:786:ASN:HA	1.50	0.94
1:B:663:LEU:CD1	1:B:703:GLN:HE22	1.74	0.93
1:C:237:SER:HA	1:C:239:PHE:H	1.33	0.93
1:C:533:LEU:HD13	1:C:642:THR:HG23	1.48	0.93
1:D:533:LEU:O	1:D:644:LYS:CB	2.16	0.93
1:A:805:ALA:HB1	1:A:808:ARG:H	1.30	0.93
1:A:816:LYS:HE3	1:A:910:ILE:CG2	1.98	0.93
1:D:534:HIS:HD2	1:D:644:LYS:NZ	1.66	0.93
1:A:237:SER:HA	1:A:239:PHE:H	1.33	0.92
1:D:663:LEU:HD12	1:D:792:ASP:HB2	1.50	0.92
1:C:702:PRO:CB	1:C:728:PRO:HD3	1.99	0.92
1:B:778:ALA:CB	1:B:798:LYS:HD2	2.00	0.92
1:B:795:GLN:HB2	1:B:797:LEU:CD1	1.99	0.92
1:D:237:SER:HA	1:D:239:PHE:H	1.33	0.92
1:C:778:ALA:CB	1:C:798:LYS:HD2	2.00	0.92
1:A:735:ARG:HG2	1:A:786:ASN:HA	1.50	0.92
1:A:795:GLN:HB2	1:A:797:LEU:CD1	1.99	0.92
1:D:533:LEU:HD13	1:D:642:THR:CG2	1.92	0.92
1:C:795:GLN:HB2	1:C:797:LEU:CD1	1.99	0.91
1:B:549:ALA:O	1:B:586:PRO:CA	2.18	0.91
1:D:533:LEU:HB3	1:D:642:THR:CB	2.00	0.91
1:D:795:GLN:HB2	1:D:797:LEU:CD1	1.99	0.91
1:A:655:ASN:OD1	1:A:657:SER:HB2	1.71	0.91
1:A:778:ALA:CB	1:A:798:LYS:HD2	2.00	0.91
1:D:534:HIS:HD2	1:D:644:LYS:HZ3	0.94	0.91
1:D:663:LEU:HD11	1:D:792:ASP:CG	1.94	0.91
1:C:702:PRO:HB3	1:C:728:PRO:CD	2.01	0.90
1:B:775:SER:H	1:B:807:GLN:CD	1.79	0.90
1:D:737:TYR:CE1	1:D:754:ARG:HD2	2.06	0.90
1:B:692:GLU:OE2	1:D:141:ARG:NH1	2.05	0.90
1:C:737:TYR:CE1	1:C:754:ARG:HD2	2.06	0.90
1:A:737:TYR:CE1	1:A:754:ARG:HD2	2.06	0.90
1:B:707:THR:HG21	1:B:723:LYS:HD3	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:TYR:CE1	1:B:754:ARG:HD2	2.06	0.90
1:A:422:LEU:CD1	1:B:605:GLN:CG	2.49	0.90
1:A:655:ASN:HB3	1:A:658:ALA:CB	2.02	0.90
1:A:816:LYS:CE	1:A:910:ILE:HG23	2.02	0.89
1:C:533:LEU:CD1	1:C:642:THR:HG23	2.01	0.89
1:D:778:ALA:CB	1:D:798:LYS:HD2	2.00	0.89
1:A:655:ASN:C	1:A:656:CYS:CA	2.44	0.89
1:A:707:THR:HG21	1:A:723:LYS:HD3	1.54	0.89
1:C:663:LEU:CD1	1:C:792:ASP:CG	2.44	0.89
1:B:533:LEU:HA	1:B:646:PHE:HB2	1.54	0.89
1:B:706:PRO:HA	1:B:797:LEU:HD21	1.55	0.89
1:C:707:THR:HG21	1:C:723:LYS:HD3	1.54	0.89
1:A:655:ASN:C	1:A:658:ALA:H	1.80	0.88
1:A:810:SER:CB	1:A:882:ASN:OD1	2.22	0.88
1:A:508:VAL:C	1:A:509:GLU:N	0.78	0.88
1:C:533:LEU:HD22	1:C:639:SER:CB	2.04	0.88
1:A:932:LEU:HB3	1:A:943:THR:CG2	2.04	0.88
1:D:663:LEU:HD12	1:D:792:ASP:CG	1.99	0.87
1:C:663:LEU:HD12	1:C:792:ASP:CB	2.04	0.87
1:C:893:HIS:HB2	1:C:933:CYS:O	1.75	0.87
1:A:655:ASN:O	1:A:658:ALA:CB	2.21	0.87
1:C:959:LEU:CD1	1:C:1033:LEU:HD23	2.04	0.87
1:D:533:LEU:HD12	1:D:642:THR:CG2	1.91	0.87
1:D:550:ASN:HB2	1:D:586:PRO:HB3	0.89	0.87
1:D:707:THR:HG21	1:D:723:LYS:HD3	1.54	0.87
1:D:959:LEU:CD1	1:D:1033:LEU:HD23	2.04	0.87
1:B:533:LEU:HA	1:B:646:PHE:CB	2.04	0.87
1:A:549:ALA:O	1:A:586:PRO:HB3	1.74	0.87
1:D:893:HIS:HB2	1:D:933:CYS:O	1.75	0.87
1:D:551:ARG:NH2	1:D:642:THR:HG22	1.89	0.87
1:A:810:SER:HB2	1:A:882:ASN:ND2	1.89	0.86
1:D:932:LEU:HB3	1:D:943:THR:CG2	2.04	0.86
1:A:706:PRO:HA	1:A:797:LEU:HD21	1.55	0.86
1:C:706:PRO:HA	1:C:797:LEU:HD21	1.55	0.86
1:D:706:PRO:HA	1:D:797:LEU:HD21	1.55	0.86
1:D:711:LEU:HD23	1:D:821:PHE:CD1	2.10	0.86
1:C:934:ILE:HD12	1:C:941:PHE:HD1	1.40	0.86
1:D:550:ASN:CB	1:D:586:PRO:CB	2.39	0.86
1:A:655:ASN:C	1:A:656:CYS:C	2.43	0.86
1:C:932:LEU:HB3	1:C:943:THR:CG2	2.04	0.86
1:B:533:LEU:CD2	1:B:646:PHE:CD2	2.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:934:ILE:HD12	1:D:941:PHE:HD1	1.40	0.85
1:D:550:ASN:ND2	1:D:586:PRO:HA	1.91	0.85
1:D:775:SER:HB3	1:D:807:GLN:HG3	1.59	0.85
1:A:893:HIS:HB2	1:A:933:CYS:O	1.75	0.85
1:A:934:ILE:HD12	1:A:941:PHE:HD1	1.40	0.85
1:B:701:CYS:C	1:B:702:PRO:N	2.35	0.85
1:A:422:LEU:HD12	1:B:605:GLN:CD	2.01	0.85
1:C:533:LEU:HD22	1:C:639:SER:HB2	1.57	0.84
1:D:775:SER:CB	1:D:807:GLN:CG	2.55	0.84
1:B:743:ILE:HB	1:B:746:ALA:O	1.78	0.84
1:D:551:ARG:NH1	1:D:641:GLU:CD	2.35	0.84
1:C:743:ILE:HB	1:C:746:ALA:O	1.78	0.84
1:B:702:PRO:HB3	1:B:726:ASN:O	1.76	0.83
1:C:795:GLN:HB2	1:C:797:LEU:HD12	1.60	0.83
1:D:743:ILE:HB	1:D:746:ALA:O	1.78	0.83
1:D:803:LYS:C	1:D:804:CYS:O	2.17	0.83
1:A:407:LEU:CD2	1:C:944:LYS:CE	2.56	0.83
1:C:818:ASP:HB2	1:C:821:PHE:CD2	2.14	0.83
1:B:818:ASP:HB2	1:B:821:PHE:CD2	2.14	0.83
1:A:301:THR:HG21	1:B:589:SER:HB2	1.60	0.83
1:A:743:ILE:HB	1:A:746:ALA:O	1.78	0.83
1:C:893:HIS:CE1	1:C:894:VAL:HG22	2.14	0.83
1:A:818:ASP:HB2	1:A:821:PHE:CD2	2.14	0.82
1:B:795:GLN:HB2	1:B:797:LEU:HD12	1.60	0.82
1:A:893:HIS:CE1	1:A:894:VAL:HG22	2.14	0.82
1:D:663:LEU:HD11	1:D:792:ASP:OD2	1.78	0.82
1:D:893:HIS:CE1	1:D:894:VAL:HG22	2.14	0.82
1:D:550:ASN:HD22	1:D:586:PRO:CA	1.93	0.82
1:D:534:HIS:CD2	1:D:644:LYS:NZ	2.43	0.82
1:D:818:ASP:HB2	1:D:821:PHE:CD2	2.14	0.82
1:A:893:HIS:HD1	1:A:932:LEU:HA	1.44	0.81
1:D:795:GLN:HB2	1:D:797:LEU:HD12	1.60	0.81
1:A:795:GLN:HB2	1:A:797:LEU:HD12	1.60	0.81
1:A:816:LYS:HE3	1:A:910:ILE:HG23	1.61	0.81
1:C:907:GLU:OE1	1:C:915:VAL:HG11	1.81	0.81
1:A:407:LEU:HD23	1:C:944:LYS:CD	1.96	0.81
1:B:741:LEU:O	1:B:747:VAL:HG23	1.81	0.81
1:B:711:LEU:HD21	1:B:820:LYS:HB3	1.62	0.81
1:C:893:HIS:HD1	1:C:932:LEU:HA	1.44	0.81
1:A:907:GLU:OE1	1:A:915:VAL:HG11	1.81	0.81
1:C:735:ARG:CG	1:C:786:ASN:HA	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:893:HIS:HD1	1:D:932:LEU:HA	1.44	0.81
1:D:741:LEU:O	1:D:747:VAL:HG23	1.81	0.81
1:D:907:GLU:OE1	1:D:915:VAL:HG11	1.81	0.81
1:B:802:TYR:CG	1:B:821:PHE:CD1	2.69	0.80
1:C:741:LEU:O	1:C:747:VAL:HG23	1.81	0.80
1:C:883:LEU:HB2	1:C:911:ALA:HA	1.63	0.80
1:D:735:ARG:CG	1:D:786:ASN:HA	2.11	0.80
1:A:784:VAL:HG22	1:A:790:ILE:HG22	1.63	0.80
1:C:677:TYR:CD1	1:C:731:GLN:CG	2.63	0.80
1:D:803:LYS:O	1:D:804:CYS:C	2.16	0.80
1:D:883:LEU:HB2	1:D:911:ALA:HA	1.63	0.80
1:B:559:CYS:C	1:B:560:MET:N	2.40	0.80
1:B:735:ARG:CG	1:B:786:ASN:HA	2.11	0.80
1:D:904:ILE:CG2	1:D:907:GLU:HB2	2.12	0.80
1:A:904:ILE:CG2	1:A:907:GLU:HB2	2.12	0.80
1:B:692:GLU:OE2	1:D:141:ARG:CZ	2.29	0.80
1:B:784:VAL:HG22	1:B:790:ILE:HG22	1.63	0.80
1:D:775:SER:HB2	1:D:807:GLN:CG	2.12	0.80
1:A:735:ARG:CG	1:A:786:ASN:HA	2.11	0.80
1:C:904:ILE:CG2	1:C:907:GLU:HB2	2.12	0.80
1:C:893:HIS:CE1	1:C:932:LEU:HG	2.18	0.79
1:D:812:GLY:HA3	1:D:885:LEU:CD2	2.11	0.79
1:A:217:LEU:HD11	1:C:940:GLU:OE1	1.83	0.79
1:A:397:PRO:HB2	1:C:947:GLN:NE2	1.95	0.79
1:D:784:VAL:HG22	1:D:790:ILE:HG22	1.63	0.79
1:A:407:LEU:HD21	1:C:944:LYS:HD2	0.79	0.79
1:A:741:LEU:O	1:A:747:VAL:HG23	1.81	0.79
1:B:690:PHE:HE2	1:B:731:GLN:HB3	1.47	0.79
1:B:775:SER:CB	1:B:807:GLN:OE1	2.30	0.79
1:B:663:LEU:CD1	1:B:703:GLN:HE21	1.96	0.79
1:C:784:VAL:HG22	1:C:790:ILE:HG22	1.63	0.79
1:D:533:LEU:CD1	1:D:639:SER:OG	2.31	0.79
1:D:893:HIS:CE1	1:D:932:LEU:HG	2.18	0.78
1:A:463:PRO:HD2	1:B:577:LEU:HD22	1.65	0.78
1:B:550:ASN:HB2	1:B:585:ALA:C	2.08	0.78
1:D:663:LEU:CD1	1:D:792:ASP:CB	2.56	0.78
1:D:823:CYS:HA	1:D:834:LEU:HD23	1.65	0.78
1:A:422:LEU:HD12	1:B:605:GLN:CG	2.14	0.78
1:C:823:CYS:HA	1:C:834:LEU:HD23	1.65	0.78
1:D:958:SER:HA	1:D:1033:LEU:CD2	2.13	0.78
1:A:463:PRO:HG2	1:B:612:ILE:HB	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:812:GLY:CA	1:D:885:LEU:CD2	2.62	0.78
1:A:893:HIS:CE1	1:A:932:LEU:HG	2.18	0.78
1:A:883:LEU:HB2	1:A:911:ALA:HA	1.63	0.77
1:A:737:TYR:HE1	1:A:754:ARG:HD2	1.50	0.77
1:B:550:ASN:HB2	1:B:586:PRO:CA	2.13	0.77
1:A:890:ILE:HD13	1:A:908:TYR:CE1	2.20	0.77
1:D:786:ASN:HB3	1:D:789:PHE:HD2	1.50	0.77
1:D:795:GLN:HB2	1:D:797:LEU:HD11	1.67	0.77
1:B:533:LEU:HD22	1:B:646:PHE:CG	2.00	0.77
1:B:823:CYS:HA	1:B:834:LEU:HD23	1.65	0.77
1:D:890:ILE:HD13	1:D:908:TYR:CE1	2.20	0.77
1:B:775:SER:HB2	1:B:807:GLN:CD	2.08	0.77
1:D:729:GLN:HG3	1:D:754:ARG:NH1	2.00	0.76
1:A:795:GLN:HB2	1:A:797:LEU:HD11	1.67	0.76
1:A:823:CYS:HA	1:A:834:LEU:HD23	1.65	0.76
1:C:795:GLN:HB2	1:C:797:LEU:HD11	1.67	0.76
1:D:533:LEU:HB3	1:D:642:THR:OG1	1.86	0.76
1:A:786:ASN:HB3	1:A:789:PHE:HD2	1.50	0.76
1:C:729:GLN:HG3	1:C:754:ARG:NH1	2.00	0.76
1:B:550:ASN:HB2	1:B:586:PRO:N	1.99	0.76
1:D:812:GLY:CA	1:D:885:LEU:HD21	2.16	0.76
1:A:815:LEU:HD23	1:A:853:VAL:CG1	2.15	0.76
1:C:786:ASN:HB3	1:C:789:PHE:HD2	1.50	0.76
1:C:958:SER:HA	1:C:1033:LEU:CD2	2.13	0.76
1:B:729:GLN:HG3	1:B:754:ARG:NH1	2.00	0.76
1:C:890:ILE:HD13	1:C:908:TYR:CE1	2.20	0.76
1:A:463:PRO:CG	1:B:612:ILE:HG21	2.00	0.76
1:B:775:SER:CB	1:B:807:GLN:CD	2.59	0.75
1:D:440:TYR:CE2	1:D:527:HIS:HA	2.21	0.75
1:D:737:TYR:HE1	1:D:754:ARG:HD2	1.50	0.75
1:A:729:GLN:HG3	1:A:754:ARG:NH1	2.00	0.75
1:B:795:GLN:HB2	1:B:797:LEU:HD11	1.67	0.75
1:D:996:PHE:HZ	1:D:999:ARG:HB2	1.51	0.75
1:C:996:PHE:HZ	1:C:999:ARG:HB2	1.51	0.75
1:C:960:SER:OG	1:C:973:THR:HB	1.86	0.75
1:C:707:THR:CG2	1:C:723:LYS:HD3	2.17	0.75
1:A:655:ASN:CG	1:A:658:ALA:N	2.45	0.75
1:C:896:VAL:HG21	1:C:918:MET:HE3	1.68	0.75
1:B:786:ASN:HB3	1:B:789:PHE:HD2	1.50	0.75
1:B:802:TYR:CD2	1:B:821:PHE:CD1	2.75	0.75
1:C:737:TYR:HE1	1:C:754:ARG:HD2	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:PRO:O	1:A:921:ALA:HB3	1.87	0.75
1:D:870:PRO:O	1:D:921:ALA:HB3	1.87	0.75
1:D:815:LEU:HD23	1:D:853:VAL:CG1	2.15	0.74
1:D:960:SER:OG	1:D:973:THR:HB	1.86	0.74
1:A:896:VAL:HG21	1:A:918:MET:HE3	1.68	0.74
1:B:459:ARG:NH1	1:B:524:GLY:O	2.20	0.74
1:D:707:THR:CG2	1:D:723:LYS:HD3	2.17	0.74
1:B:470:TYR:CE1	1:B:525:ASP:CG	2.66	0.74
1:B:775:SER:CA	1:B:807:GLN:OE1	2.36	0.74
1:A:815:LEU:CB	1:A:885:LEU:HD11	2.17	0.74
1:D:714:VAL:HG13	1:D:767:TYR:O	1.88	0.74
1:A:714:VAL:HG13	1:A:767:TYR:O	1.88	0.73
1:B:707:THR:CG2	1:B:723:LYS:HD3	2.17	0.73
1:B:714:VAL:HG13	1:B:767:TYR:O	1.88	0.73
1:C:873:GLY:HA3	1:C:1026:ARG:HG3	1.70	0.73
1:C:870:PRO:O	1:C:921:ALA:HB3	1.87	0.73
1:A:893:HIS:ND1	1:A:932:LEU:HA	2.02	0.73
1:C:714:VAL:HG13	1:C:767:TYR:O	1.88	0.73
1:C:445:VAL:HG22	1:C:526:PRO:HG2	1.70	0.73
1:D:896:VAL:HG21	1:D:918:MET:HE3	1.69	0.73
1:A:707:THR:CG2	1:A:723:LYS:HD3	2.17	0.73
1:D:533:LEU:HD21	1:D:639:SER:CB	2.07	0.73
1:B:533:LEU:HD23	1:B:646:PHE:CB	2.19	0.73
1:D:893:HIS:ND1	1:D:932:LEU:HA	2.02	0.73
1:D:997:TYR:HB3	1:D:1005:VAL:HG23	1.70	0.73
1:C:893:HIS:ND1	1:C:932:LEU:HA	2.02	0.73
1:C:997:TYR:HB3	1:C:1005:VAL:HG23	1.70	0.73
1:D:550:ASN:HB2	1:D:586:PRO:CA	2.18	0.73
1:D:786:ASN:HB3	1:D:789:PHE:CD2	2.24	0.72
1:A:702:PRO:O	1:A:703:GLN:CB	2.35	0.72
1:B:786:ASN:HB3	1:B:789:PHE:CD2	2.24	0.72
1:B:544:GLN:HG2	1:B:545:ARG:HG2	1.71	0.72
1:B:550:ASN:CB	1:B:585:ALA:C	2.63	0.72
1:C:1018:VAL:O	1:C:1034:GLN:HG3	1.88	0.72
1:D:1018:VAL:O	1:D:1034:GLN:HG3	1.88	0.72
1:B:533:LEU:HD21	1:B:646:PHE:CD1	2.24	0.72
1:C:663:LEU:HD12	1:C:792:ASP:HB3	1.72	0.72
1:D:988:TYR:HB3	1:D:1021:SER:HB3	1.70	0.72
1:A:863:ILE:CD1	1:A:878:ILE:HG12	2.20	0.72
1:D:775:SER:HB3	1:D:807:GLN:CG	2.18	0.72
1:A:655:ASN:O	1:A:658:ALA:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:872:GLY:O	1:C:1026:ARG:HB2	1.89	0.71
1:A:422:LEU:HD12	1:B:605:GLN:HG2	1.66	0.71
1:C:988:TYR:HB3	1:C:1021:SER:HB3	1.71	0.71
1:D:893:HIS:NE2	1:D:914:ILE:HD13	2.05	0.71
1:A:786:ASN:HB3	1:A:789:PHE:CD2	2.24	0.71
1:A:883:LEU:HD23	1:A:914:ILE:HD11	1.72	0.71
1:C:863:ILE:CD1	1:C:878:ILE:HG12	2.20	0.71
1:C:893:HIS:NE2	1:C:914:ILE:HD13	2.05	0.71
1:D:883:LEU:HD23	1:D:914:ILE:HD11	1.72	0.71
1:B:711:LEU:CD2	1:B:820:LYS:HB3	2.20	0.71
1:B:732:SER:HB2	1:D:83:HIS:NE2	2.04	0.71
1:C:815:LEU:HD23	1:C:853:VAL:CG1	2.15	0.71
1:D:560:MET:HE2	1:D:586:PRO:HD3	1.73	0.71
1:A:810:SER:HB2	1:A:882:ASN:HD21	1.53	0.71
1:C:786:ASN:HB3	1:C:789:PHE:CD2	2.24	0.71
1:A:893:HIS:NE2	1:A:914:ILE:HD13	2.05	0.71
1:D:855:CYS:SG	1:D:885:LEU:HD21	2.30	0.71
1:A:221:PHE:CZ	1:C:830:ARG:HB2	2.25	0.71
1:B:549:ALA:O	1:B:586:PRO:HA	1.91	0.71
1:C:560:MET:HE2	1:C:586:PRO:HD3	1.73	0.71
1:B:737:TYR:HE1	1:B:754:ARG:HD2	1.50	0.71
1:A:655:ASN:CA	1:A:656:CYS:N	2.54	0.70
1:C:544:GLN:HG2	1:C:545:ARG:HG2	1.71	0.70
1:D:544:GLN:HG2	1:D:545:ARG:HG2	1.71	0.70
1:A:544:GLN:HG2	1:A:545:ARG:HG2	1.71	0.70
1:A:920:HIS:NE2	1:A:922:VAL:HG23	2.06	0.70
1:C:855:CYS:C	1:C:856:SER:N	2.48	0.70
1:D:863:ILE:CD1	1:D:878:ILE:HG12	2.20	0.70
1:D:920:HIS:NE2	1:D:922:VAL:HG23	2.06	0.70
1:B:690:PHE:HE2	1:B:731:GLN:CB	2.03	0.70
1:B:697:VAL:HG12	1:B:699:GLU:H	1.57	0.70
1:B:803:LYS:C	1:B:804:CYS:CA	2.65	0.70
1:C:920:HIS:NE2	1:C:922:VAL:HG23	2.06	0.70
1:A:407:LEU:HD23	1:C:944:LYS:HZ2	1.55	0.70
1:A:811:CYS:O	1:A:815:LEU:HD13	1.92	0.70
1:A:838:CYS:SG	1:A:839:PRO:HD2	2.32	0.70
1:B:815:LEU:HD23	1:B:853:VAL:CG1	2.15	0.70
1:C:697:VAL:HG12	1:C:699:GLU:H	1.57	0.70
1:C:811:CYS:O	1:C:815:LEU:HD13	1.92	0.70
1:C:883:LEU:HD23	1:C:914:ILE:HD11	1.72	0.70
1:D:838:CYS:SG	1:D:839:PRO:HD2	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:THR:CG2	1:B:837:HIS:HB2	2.22	0.70
1:C:774:ILE:C	1:C:806:ALA:HB3	2.15	0.70
1:D:811:CYS:O	1:D:815:LEU:HD13	1.92	0.70
1:A:697:VAL:HG12	1:A:699:GLU:H	1.56	0.70
1:D:938:LYS:HB2	1:D:941:PHE:HD2	1.57	0.70
1:B:838:CYS:SG	1:B:839:PRO:HD2	2.32	0.69
1:C:938:LYS:HB2	1:C:941:PHE:HD2	1.57	0.69
1:A:868:GLY:HA3	1:A:949:TYR:OH	1.92	0.69
1:B:811:CYS:O	1:B:815:LEU:HD13	1.92	0.69
1:C:818:ASP:HB2	1:C:821:PHE:CE2	2.28	0.69
1:D:697:VAL:HG12	1:D:699:GLU:H	1.57	0.69
1:A:810:SER:CB	1:A:882:ASN:HD21	2.06	0.69
1:B:560:MET:HE2	1:B:586:PRO:HD3	1.73	0.69
1:A:870:PRO:HD3	1:A:952:VAL:O	1.92	0.69
1:D:533:LEU:HD11	1:D:639:SER:OG	1.91	0.69
1:A:560:MET:HE2	1:A:586:PRO:HD3	1.73	0.69
1:A:818:ASP:HB2	1:A:821:PHE:CE2	2.28	0.69
1:A:833:THR:CG2	1:A:837:HIS:HB2	2.22	0.69
1:A:938:LYS:HB2	1:A:941:PHE:HD2	1.57	0.69
1:C:663:LEU:CD1	1:C:792:ASP:CB	2.69	0.69
1:C:838:CYS:SG	1:C:839:PRO:HD2	2.32	0.69
1:C:868:GLY:HA3	1:C:949:TYR:OH	1.92	0.69
1:D:818:ASP:HB2	1:D:821:PHE:CE2	2.28	0.69
1:A:463:PRO:CG	1:B:612:ILE:HB	2.23	0.69
1:B:818:ASP:HB2	1:B:821:PHE:CE2	2.28	0.69
1:C:833:THR:CG2	1:C:837:HIS:HB2	2.22	0.69
1:C:870:PRO:HD3	1:C:952:VAL:O	1.92	0.69
1:D:550:ASN:HB3	1:D:586:PRO:HG3	1.73	0.69
1:D:868:GLY:HA3	1:D:949:TYR:OH	1.92	0.69
1:A:893:HIS:NE2	1:A:894:VAL:HG22	2.08	0.69
1:B:692:GLU:CD	1:D:141:ARG:NH2	2.42	0.69
1:D:870:PRO:HD3	1:D:952:VAL:O	1.93	0.69
1:A:815:LEU:HB3	1:A:885:LEU:HD11	1.74	0.69
1:D:833:THR:CG2	1:D:837:HIS:HB2	2.22	0.69
1:D:663:LEU:CD1	1:D:792:ASP:HB2	2.23	0.68
1:D:893:HIS:NE2	1:D:894:VAL:HG22	2.08	0.68
1:A:740:VAL:HG22	1:A:749:ARG:HD2	1.76	0.68
1:A:815:LEU:HA	1:A:848:TRP:CD1	2.29	0.68
1:A:890:ILE:HB	1:A:893:HIS:HD2	1.58	0.68
1:D:890:ILE:HB	1:D:893:HIS:HD2	1.59	0.68
1:A:79:ILE:HD11	1:A:82:ALA:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:ASN:CB	1:C:586:PRO:HB3	2.24	0.68
1:D:79:ILE:HD11	1:D:82:ALA:HB2	1.75	0.68
1:B:815:LEU:HA	1:B:848:TRP:CD1	2.29	0.68
1:C:79:ILE:HD11	1:C:82:ALA:HB2	1.75	0.68
1:C:890:ILE:HB	1:C:893:HIS:HD2	1.59	0.68
1:A:508:VAL:O	1:A:509:GLU:CA	2.29	0.68
1:B:737:TYR:CD2	1:B:785:TRP:HB3	2.29	0.68
1:C:737:TYR:CD2	1:C:785:TRP:HB3	2.29	0.68
1:D:564:VAL:HG22	1:D:580:LEU:HD13	1.76	0.68
1:D:815:LEU:HA	1:D:848:TRP:CD1	2.29	0.68
1:D:737:TYR:CD2	1:D:785:TRP:HB3	2.29	0.68
1:D:988:TYR:HE1	1:D:992:GLN:C	2.02	0.68
1:A:704:LEU:HD11	1:A:783:VAL:CG2	2.24	0.68
1:B:655:ASN:C	1:B:656:CYS:CA	2.66	0.68
1:C:988:TYR:HE1	1:C:992:GLN:C	2.02	0.68
1:A:706:PRO:CA	1:A:797:LEU:HD21	2.24	0.68
1:B:79:ILE:HD11	1:B:82:ALA:HB2	1.75	0.68
1:B:810:SER:OG	1:B:813:LEU:HD13	1.94	0.68
1:C:810:SER:OG	1:C:813:LEU:HD13	1.94	0.68
1:B:740:VAL:HG22	1:B:749:ARG:HD2	1.75	0.67
1:D:704:LEU:HD11	1:D:783:VAL:CG2	2.24	0.67
1:C:704:LEU:HD11	1:C:783:VAL:CG2	2.24	0.67
1:C:713:PRO:HG3	1:C:802:TYR:OH	1.95	0.67
1:B:704:LEU:HD11	1:B:783:VAL:CG2	2.24	0.67
1:B:713:PRO:HG3	1:B:802:TYR:OH	1.95	0.67
1:C:564:VAL:HG22	1:C:580:LEU:HD13	1.76	0.67
1:C:863:ILE:HG13	1:C:877:THR:O	1.94	0.67
1:A:863:ILE:HG13	1:A:877:THR:O	1.95	0.67
1:D:713:PRO:HG3	1:D:802:TYR:OH	1.95	0.67
1:C:815:LEU:HA	1:C:848:TRP:CD1	2.29	0.67
1:D:810:SER:OG	1:D:813:LEU:HD13	1.94	0.67
1:D:1015:LEU:H	1:D:1015:LEU:HD12	1.59	0.67
1:A:737:TYR:CD2	1:A:785:TRP:HB3	2.29	0.67
1:A:810:SER:OG	1:A:813:LEU:HD13	1.94	0.67
1:B:568:SER:HG	1:B:670:PHE:HD1	1.41	0.67
1:A:463:PRO:CD	1:B:612:ILE:HG21	2.24	0.67
1:C:893:HIS:NE2	1:C:894:VAL:HG22	2.08	0.67
1:D:740:VAL:HG22	1:D:749:ARG:HD2	1.76	0.67
1:B:564:VAL:HG22	1:B:580:LEU:HD13	1.76	0.67
1:B:703:GLN:HA	1:B:792:ASP:OD1	1.95	0.67
1:C:655:ASN:OD1	1:C:657:SER:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1015:LEU:H	1:C:1015:LEU:HD12	1.59	0.67
1:B:666:VAL:HG11	1:B:698:SER:N	2.10	0.67
1:B:805:ALA:HB1	1:B:808:ARG:N	2.08	0.67
1:B:237:SER:HA	1:B:239:PHE:N	2.07	0.66
1:B:690:PHE:CD2	1:B:731:GLN:HG3	2.30	0.66
1:C:740:VAL:HG22	1:C:749:ARG:HD2	1.75	0.66
1:A:564:VAL:HG22	1:A:580:LEU:HD13	1.76	0.66
1:B:706:PRO:CA	1:B:797:LEU:HD21	2.24	0.66
1:C:559:CYS:O	1:C:584:ASP:CB	2.43	0.66
1:C:702:PRO:HA	1:C:726:ASN:O	1.95	0.66
1:C:533:LEU:CD2	1:C:639:SER:HB2	2.23	0.66
1:C:956:VAL:HG23	1:C:975:THR:O	1.95	0.66
1:D:666:VAL:HG11	1:D:698:SER:N	2.10	0.66
1:D:956:VAL:HG23	1:D:975:THR:O	1.95	0.66
1:B:714:VAL:HG13	1:B:768:GLN:HA	1.77	0.66
1:D:703:GLN:HA	1:D:792:ASP:OD1	1.95	0.66
1:D:863:ILE:HG13	1:D:877:THR:O	1.94	0.66
1:A:706:PRO:HG3	1:A:795:GLN:HG3	1.78	0.66
1:B:533:LEU:HD21	1:B:646:PHE:CE1	2.31	0.66
1:C:677:TYR:HD1	1:C:731:GLN:HG3	1.55	0.66
1:C:706:PRO:CA	1:C:797:LEU:HD21	2.24	0.66
1:A:324:GLN:HE21	1:B:577:LEU:H	1.42	0.66
1:A:713:PRO:HG3	1:A:802:TYR:OH	1.95	0.66
1:C:237:SER:HA	1:C:239:PHE:N	2.08	0.66
1:D:717:VAL:CG1	1:D:764:ASN:HB3	2.26	0.66
1:A:714:VAL:HG13	1:A:768:GLN:HA	1.78	0.66
1:B:717:VAL:CG1	1:B:764:ASN:HB3	2.26	0.66
1:B:732:SER:CB	1:D:83:HIS:CD2	2.78	0.66
1:C:714:VAL:HG13	1:C:768:GLN:HA	1.77	0.66
1:B:802:TYR:CD1	1:B:821:PHE:CD1	2.84	0.66
1:D:793:ASN:OD1	1:D:797:LEU:HD13	1.96	0.66
1:A:237:SER:HA	1:A:239:PHE:N	2.08	0.66
1:C:1015:LEU:HD21	1:C:1039:ASP:HB2	1.78	0.65
1:A:666:VAL:HG11	1:A:698:SER:N	2.10	0.65
1:A:703:GLN:HA	1:A:792:ASP:OD1	1.95	0.65
1:B:551:ARG:NH2	1:B:642:THR:HG21	2.11	0.65
1:C:666:VAL:HG11	1:C:698:SER:N	2.10	0.65
1:C:703:GLN:HA	1:C:792:ASP:OD1	1.95	0.65
1:C:717:VAL:CG1	1:C:764:ASN:HB3	2.26	0.65
1:C:793:ASN:OD1	1:C:797:LEU:HD13	1.96	0.65
1:D:237:SER:HA	1:D:239:PHE:N	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:CYS:O	1:A:703:GLN:HG3	1.95	0.65
1:D:706:PRO:CA	1:D:797:LEU:HD21	2.24	0.65
1:D:1015:LEU:HD21	1:D:1039:ASP:HB2	1.78	0.65
1:B:711:LEU:HD21	1:B:820:LYS:CB	2.25	0.65
1:A:717:VAL:CG1	1:A:764:ASN:HB3	2.26	0.65
1:B:793:ASN:OD1	1:B:797:LEU:HD13	1.96	0.65
1:D:864:LEU:HG	1:D:865:THR:N	2.12	0.65
1:D:812:GLY:CA	1:D:885:LEU:HD22	2.26	0.65
1:D:714:VAL:HG13	1:D:768:GLN:HA	1.78	0.65
1:A:742:SER:O	1:A:779:VAL:HG13	1.97	0.65
1:C:864:LEU:HG	1:C:865:THR:N	2.12	0.65
1:A:772:MET:O	1:A:806:ALA:HB1	1.97	0.65
1:A:864:LEU:HG	1:A:865:THR:N	2.12	0.65
1:A:931:ARG:HD2	1:A:942:MET:HE3	1.79	0.65
1:C:88:GLU:HB2	1:C:132:LEU:HD21	1.79	0.65
1:C:742:SER:O	1:C:779:VAL:HG13	1.97	0.65
1:A:88:GLU:HB2	1:A:132:LEU:HD21	1.79	0.64
1:A:793:ASN:OD1	1:A:797:LEU:HD13	1.96	0.64
1:C:931:ARG:HD2	1:C:942:MET:HE3	1.79	0.64
1:D:931:ARG:HD2	1:D:942:MET:HE3	1.79	0.64
1:D:706:PRO:HG3	1:D:795:GLN:HG3	1.78	0.64
1:A:655:ASN:OD1	1:A:658:ALA:N	2.30	0.64
1:D:88:GLU:HB2	1:D:132:LEU:HD21	1.79	0.64
1:D:742:SER:O	1:D:779:VAL:HG13	1.97	0.64
1:A:704:LEU:HD11	1:A:783:VAL:HG21	1.80	0.64
1:A:842:SER:OG	1:A:844:PRO:HD2	1.97	0.64
1:B:695:ILE:CD1	1:B:702:PRO:HD3	2.28	0.64
1:A:805:ALA:HB1	1:A:808:ARG:N	2.08	0.64
1:C:842:SER:OG	1:C:844:PRO:HD2	1.97	0.64
1:D:812:GLY:HA3	1:D:885:LEU:HD22	1.78	0.64
1:B:550:ASN:HB2	1:B:586:PRO:HA	1.80	0.64
1:C:706:PRO:HG3	1:C:795:GLN:HG3	1.78	0.64
1:A:549:ALA:O	1:A:586:PRO:CB	2.45	0.64
1:B:706:PRO:HG3	1:B:795:GLN:HG3	1.78	0.64
1:C:533:LEU:HD13	1:C:639:SER:OG	1.98	0.64
1:A:810:SER:CB	1:A:882:ASN:ND2	2.61	0.63
1:B:742:SER:O	1:B:779:VAL:HG13	1.97	0.63
1:B:533:LEU:CD2	1:B:646:PHE:CB	2.76	0.63
1:B:842:SER:OG	1:B:844:PRO:HD2	1.97	0.63
1:C:704:LEU:HD11	1:C:783:VAL:HG21	1.80	0.63
1:C:775:SER:HB2	1:C:807:GLN:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:959:LEU:HG	1:D:974:ILE:CG2	2.25	0.63
1:B:704:LEU:HD11	1:B:783:VAL:HG21	1.80	0.63
1:C:855:CYS:O	1:C:856:SER:N	2.32	0.63
1:D:842:SER:OG	1:D:844:PRO:HD2	1.97	0.63
1:B:706:PRO:HA	1:B:797:LEU:CD2	2.29	0.63
1:C:959:LEU:HG	1:C:974:ILE:CG2	2.25	0.63
1:D:470:TYR:HB2	1:D:523:SER:O	1.98	0.63
1:D:704:LEU:HD11	1:D:783:VAL:HG21	1.80	0.63
1:B:88:GLU:HB2	1:B:132:LEU:HD21	1.79	0.63
1:D:630:TRP:HB3	1:D:670:PHE:CE2	2.34	0.63
1:C:994:CYS:HA	1:C:1009:PRO:HD3	1.81	0.63
1:C:274:LEU:H	1:C:274:LEU:HD12	1.64	0.63
1:C:904:ILE:HG23	1:C:907:GLU:HB2	1.79	0.63
1:C:1001:MET:HG3	1:C:1002:ASN:N	2.13	0.63
1:D:904:ILE:HG23	1:D:907:GLU:HB2	1.79	0.63
1:D:994:CYS:HA	1:D:1009:PRO:HD3	1.81	0.63
1:C:989:LEU:HG	1:C:1020:VAL:HG12	1.81	0.62
1:D:661:LEU:HD21	1:D:790:ILE:CG1	2.28	0.62
1:D:988:TYR:C	1:D:989:LEU:HD12	2.24	0.62
1:A:274:LEU:H	1:A:274:LEU:HD12	1.64	0.62
1:A:834:LEU:HB2	1:A:837:HIS:HD2	1.64	0.62
1:B:834:LEU:HB2	1:B:837:HIS:HD2	1.64	0.62
1:C:988:TYR:C	1:C:989:LEU:HD12	2.24	0.62
1:D:989:LEU:HG	1:D:1020:VAL:HG12	1.81	0.62
1:B:663:LEU:HD12	1:B:703:GLN:HE21	1.63	0.62
1:D:274:LEU:H	1:D:274:LEU:HD12	1.64	0.62
1:D:1001:MET:HG3	1:D:1002:ASN:N	2.13	0.62
1:A:934:ILE:HD12	1:A:941:PHE:CD1	2.30	0.62
1:A:895:GLN:HG2	1:A:931:ARG:HB3	1.82	0.62
1:C:790:ILE:HG13	1:C:790:ILE:O	2.00	0.62
1:C:885:LEU:HD22	1:C:910:ILE:HD11	1.81	0.62
1:D:885:LEU:CD2	1:D:910:ILE:HD11	2.30	0.62
1:A:463:PRO:CB	1:B:612:ILE:HG22	2.29	0.62
1:B:274:LEU:HD12	1:B:274:LEU:H	1.64	0.62
1:A:50:PHE:HB3	1:A:498:MET:HE2	1.82	0.61
1:A:931:ARG:CG	1:A:942:MET:HE3	2.30	0.61
1:C:805:ALA:HB1	1:C:808:ARG:N	2.08	0.61
1:A:881:VAL:HG13	1:A:882:ASN:N	2.16	0.61
1:A:885:LEU:CD2	1:A:910:ILE:HD11	2.30	0.61
1:A:885:LEU:HD22	1:A:910:ILE:HD11	1.81	0.61
1:A:904:ILE:HG23	1:A:907:GLU:HB2	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:PRO:CB	1:B:726:ASN:O	2.47	0.61
1:C:931:ARG:CG	1:C:942:MET:HE3	2.30	0.61
1:D:834:LEU:HB2	1:D:837:HIS:HD2	1.64	0.61
1:C:874:THR:HA	1:C:1025:ASP:OD2	2.00	0.61
1:C:885:LEU:CD2	1:C:910:ILE:HD11	2.30	0.61
1:D:881:VAL:HG13	1:D:882:ASN:N	2.16	0.61
1:B:550:ASN:O	1:B:586:PRO:HG3	2.00	0.61
1:C:834:LEU:HB2	1:C:837:HIS:HD2	1.64	0.61
1:D:50:PHE:HB3	1:D:498:MET:HE2	1.82	0.61
1:D:706:PRO:HA	1:D:797:LEU:CD2	2.29	0.61
1:C:706:PRO:HA	1:C:797:LEU:CD2	2.29	0.61
1:C:895:GLN:HG2	1:C:931:ARG:HB3	1.82	0.61
1:C:881:VAL:HG13	1:C:882:ASN:N	2.16	0.61
1:A:864:LEU:HG	1:A:865:THR:H	1.66	0.61
1:B:802:TYR:CZ	1:B:821:PHE:HD1	2.19	0.61
1:D:885:LEU:HD22	1:D:910:ILE:HD11	1.81	0.61
1:D:989:LEU:HD12	1:D:989:LEU:N	2.15	0.61
1:B:790:ILE:O	1:B:790:ILE:HG13	2.00	0.61
1:D:931:ARG:CG	1:D:942:MET:HE3	2.30	0.61
1:B:50:PHE:HB3	1:B:498:MET:HE2	1.82	0.60
1:B:786:ASN:HD22	1:B:789:PHE:HE2	1.48	0.60
1:D:551:ARG:NH2	1:D:642:THR:CG2	2.62	0.60
1:A:842:SER:CB	1:A:844:PRO:HD2	2.31	0.60
1:B:508:VAL:CG1	1:B:539:ARG:NH2	2.64	0.60
1:B:802:TYR:CG	1:B:821:PHE:CE1	2.89	0.60
1:D:760:VAL:HG12	1:D:761:GLN:N	2.16	0.60
1:D:1015:LEU:HD12	1:D:1015:LEU:N	2.16	0.60
1:A:815:LEU:HB2	1:A:885:LEU:HD11	1.81	0.60
1:C:661:LEU:HD21	1:C:790:ILE:HD11	1.83	0.60
1:C:842:SER:CB	1:C:844:PRO:HD2	2.31	0.60
1:A:324:GLN:NE2	1:B:577:LEU:H	2.00	0.60
1:A:533:LEU:HD23	1:A:646:PHE:CG	2.36	0.60
1:A:760:VAL:HG12	1:A:761:GLN:N	2.16	0.60
1:C:50:PHE:HB3	1:C:498:MET:HE2	1.82	0.60
1:C:191:LYS:HB3	1:C:194:TYR:HB2	1.83	0.60
1:C:989:LEU:HD12	1:C:989:LEU:N	2.15	0.60
1:C:1015:LEU:HD12	1:C:1015:LEU:N	2.16	0.60
1:D:790:ILE:O	1:D:790:ILE:HG13	2.00	0.60
1:D:842:SER:CB	1:D:844:PRO:HD2	2.31	0.60
1:A:549:ALA:O	1:A:586:PRO:HA	2.02	0.60
1:B:815:LEU:HA	1:B:848:TRP:HD1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:786:ASN:HD22	1:D:789:PHE:HE2	1.48	0.60
1:D:895:GLN:HG2	1:D:931:ARG:HB3	1.82	0.60
1:C:934:ILE:HD12	1:C:941:PHE:CD1	2.30	0.60
1:B:786:ASN:ND2	1:B:789:PHE:HE2	2.00	0.60
1:B:842:SER:CB	1:B:844:PRO:HD2	2.31	0.60
1:C:663:LEU:HD23	1:C:698:SER:HB2	1.84	0.60
1:A:706:PRO:HA	1:A:797:LEU:CD2	2.29	0.60
1:A:790:ILE:O	1:A:790:ILE:HG13	2.00	0.60
1:B:760:VAL:HG12	1:B:761:GLN:N	2.16	0.60
1:B:815:LEU:HB3	1:B:848:TRP:HB3	1.84	0.60
1:C:786:ASN:HD22	1:C:789:PHE:HE2	1.48	0.60
1:D:191:LYS:HB3	1:D:194:TYR:HB2	1.83	0.60
1:A:550:ASN:ND2	1:A:585:ALA:O	2.29	0.59
1:C:864:LEU:HG	1:C:865:THR:H	1.66	0.59
1:D:533:LEU:CG	1:D:642:THR:CG2	2.80	0.59
1:A:786:ASN:HD22	1:A:789:PHE:HE2	1.48	0.59
1:D:550:ASN:HB3	1:D:586:PRO:CG	2.32	0.59
1:D:551:ARG:HH12	1:D:641:GLU:CD	2.06	0.59
1:D:805:ALA:HB1	1:D:808:ARG:N	2.08	0.59
1:B:191:LYS:HB3	1:B:194:TYR:HB2	1.83	0.59
1:D:663:LEU:HD23	1:D:698:SER:HB2	1.84	0.59
1:D:786:ASN:ND2	1:D:789:PHE:HE2	2.00	0.59
1:A:191:LYS:HB3	1:A:194:TYR:HB2	1.83	0.59
1:C:760:VAL:HG12	1:C:761:GLN:N	2.16	0.59
1:A:786:ASN:ND2	1:A:789:PHE:HE2	2.00	0.59
1:A:855:CYS:SG	1:A:856:SER:N	2.75	0.59
1:C:815:LEU:HA	1:C:848:TRP:HD1	1.66	0.59
1:A:655:ASN:OD1	1:A:657:SER:CB	2.45	0.59
1:B:802:TYR:CE2	1:B:821:PHE:HD1	2.19	0.59
1:C:663:LEU:HD12	1:C:792:ASP:OD2	1.95	0.59
1:D:815:LEU:HB3	1:D:848:TRP:HB3	1.84	0.59
1:A:97:PRO:HG2	1:A:158:TYR:CE1	2.38	0.59
1:B:663:LEU:HD23	1:B:698:SER:HB2	1.84	0.59
1:B:802:TYR:CD1	1:B:821:PHE:CE1	2.90	0.59
1:D:97:PRO:HG2	1:D:158:TYR:CE1	2.38	0.59
1:D:864:LEU:HG	1:D:865:THR:H	1.66	0.59
1:C:959:LEU:HD13	1:C:1033:LEU:CD2	2.26	0.59
1:D:887:PHE:O	1:D:890:ILE:HG12	2.02	0.59
1:C:97:PRO:HG2	1:C:158:TYR:CE1	2.38	0.58
1:C:703:GLN:HG2	1:C:792:ASP:OD1	2.03	0.58
1:C:887:PHE:O	1:C:890:ILE:HG12	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:VAL:HG22	1:D:526:PRO:HG2	1.85	0.58
1:D:775:SER:HB3	1:D:807:GLN:CD	2.28	0.58
1:B:459:ARG:CD	1:B:526:PRO:HG3	2.33	0.58
1:B:803:LYS:CA	1:B:804:CYS:N	2.65	0.58
1:D:443:TYR:HB2	1:D:526:PRO:HB3	1.85	0.58
1:A:703:GLN:HG2	1:A:792:ASP:OD1	2.03	0.58
1:C:815:LEU:HB3	1:C:848:TRP:HB3	1.84	0.58
1:A:663:LEU:HD23	1:A:698:SER:HB2	1.84	0.58
1:A:815:LEU:HB3	1:A:848:TRP:HB3	1.84	0.58
1:A:887:PHE:O	1:A:890:ILE:HG12	2.02	0.58
1:A:938:LYS:HE3	1:A:941:PHE:CD2	2.38	0.58
1:C:895:GLN:CG	1:C:931:ARG:HB3	2.33	0.58
1:A:815:LEU:HA	1:A:848:TRP:HD1	1.66	0.58
1:B:802:TYR:CE1	1:B:821:PHE:HD1	2.21	0.58
1:C:876:VAL:HG22	1:C:916:CYS:O	2.03	0.58
1:A:853:VAL:O	1:A:853:VAL:HG13	2.04	0.58
1:A:876:VAL:HG22	1:A:916:CYS:O	2.03	0.58
1:A:895:GLN:CG	1:A:931:ARG:HB3	2.33	0.58
1:B:97:PRO:HG2	1:B:158:TYR:CE1	2.38	0.58
1:A:422:LEU:HD13	1:B:605:GLN:HG2	1.78	0.58
1:B:533:LEU:HD13	1:B:639:SER:CB	2.33	0.58
1:D:876:VAL:HG22	1:D:916:CYS:O	2.04	0.58
1:D:1015:LEU:HD23	1:D:1039:ASP:N	2.18	0.58
1:D:550:ASN:HB3	1:D:586:PRO:CB	2.33	0.58
1:D:895:GLN:CG	1:D:931:ARG:HB3	2.34	0.58
1:D:938:LYS:HE3	1:D:941:PHE:CD2	2.39	0.58
1:C:1017:PRO:HB3	1:C:1034:GLN:NE2	2.19	0.58
1:D:703:GLN:HG2	1:D:792:ASP:OD1	2.03	0.58
1:D:815:LEU:CD2	1:D:853:VAL:HG11	2.23	0.58
1:D:959:LEU:HD13	1:D:1033:LEU:CD2	2.26	0.58
1:A:815:LEU:HD12	1:A:815:LEU:N	2.19	0.58
1:A:931:ARG:HD3	1:A:943:THR:O	2.04	0.58
1:C:1015:LEU:HD23	1:C:1039:ASP:N	2.18	0.58
1:D:815:LEU:HA	1:D:848:TRP:HD1	1.66	0.58
1:D:931:ARG:HD3	1:D:943:THR:O	2.04	0.58
1:D:1017:PRO:HB3	1:D:1034:GLN:NE2	2.19	0.58
1:A:700:ASP:O	1:A:702:PRO:HD3	2.04	0.57
1:B:703:GLN:HG2	1:B:792:ASP:OD1	2.03	0.57
1:C:470:TYR:CE1	1:C:525:ASP:CG	2.82	0.57
1:C:786:ASN:ND2	1:C:789:PHE:HE2	2.00	0.57
1:C:988:TYR:CE2	1:C:991:ASN:N	2.71	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:815:LEU:N	1:D:815:LEU:HD12	2.19	0.57
1:C:938:LYS:HE3	1:C:941:PHE:CD2	2.38	0.57
1:D:459:ARG:HD3	1:D:524:GLY:O	2.04	0.57
1:B:690:PHE:HD2	1:B:731:GLN:HG3	1.68	0.57
1:B:843:SER:OG	1:B:844:PRO:HD3	2.05	0.57
1:A:815:LEU:CD2	1:A:853:VAL:HG11	2.23	0.57
1:B:550:ASN:C	1:B:586:PRO:HG3	2.29	0.57
1:B:815:LEU:N	1:B:815:LEU:HD12	2.19	0.57
1:B:533:LEU:O	1:B:646:PHE:HB3	2.04	0.57
1:B:775:SER:HB3	1:B:807:GLN:OE1	2.04	0.57
1:C:815:LEU:HD12	1:C:815:LEU:N	2.20	0.57
1:D:934:ILE:HD12	1:D:941:PHE:CD1	2.30	0.57
1:D:988:TYR:CE2	1:D:991:ASN:N	2.71	0.57
1:A:175:SER:OG	1:A:178:GLU:HG2	2.04	0.57
1:C:931:ARG:HD3	1:C:943:THR:O	2.04	0.57
1:C:988:TYR:CZ	1:C:989:LEU:N	2.73	0.57
1:A:910:ILE:HG23	1:A:910:ILE:O	2.04	0.57
1:C:175:SER:OG	1:C:178:GLU:HG2	2.04	0.57
1:C:843:SER:OG	1:C:844:PRO:HD3	2.05	0.57
1:D:988:TYR:CZ	1:D:989:LEU:N	2.73	0.57
1:B:425:TYR:OH	1:B:456:LYS:HE2	2.05	0.57
1:C:550:ASN:HB2	1:C:586:PRO:HB3	1.86	0.57
1:C:853:VAL:O	1:C:853:VAL:HG13	2.04	0.57
1:D:175:SER:OG	1:D:178:GLU:HG2	2.04	0.57
1:B:802:TYR:CD2	1:B:821:PHE:HD1	2.23	0.56
1:D:533:LEU:HD13	1:D:642:THR:CB	2.35	0.56
1:D:958:SER:C	1:D:959:LEU:HD12	2.30	0.56
1:A:702:PRO:C	1:A:703:GLN:CA	2.77	0.56
1:B:853:VAL:HG13	1:B:853:VAL:O	2.04	0.56
1:C:775:SER:HB2	1:C:806:ALA:H	1.69	0.56
1:D:407:LEU:O	1:D:411:GLN:HG2	2.05	0.56
1:D:529:GLY:HA3	1:D:552:PHE:CZ	2.40	0.56
1:D:910:ILE:HG23	1:D:910:ILE:O	2.04	0.56
1:A:529:GLY:HA3	1:A:552:PHE:CZ	2.40	0.56
1:A:532:ALA:CB	1:A:560:MET:CE	2.73	0.56
1:B:533:LEU:CD2	1:B:646:PHE:CE1	2.85	0.56
1:B:663:LEU:HD12	1:B:703:GLN:NE2	2.12	0.56
1:C:425:TYR:OH	1:C:456:LYS:HE2	2.05	0.56
1:C:529:GLY:HA3	1:C:552:PHE:CZ	2.41	0.56
1:D:663:LEU:CG	1:D:792:ASP:OD2	2.53	0.56
1:D:830:ARG:O	1:D:830:ARG:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:SER:OG	1:B:178:GLU:HG2	2.04	0.56
1:C:974:ILE:HD11	1:C:1004:ILE:HB	1.88	0.56
1:D:843:SER:OG	1:D:844:PRO:HD3	2.05	0.56
1:A:420:GLU:HB3	1:B:607:SER:HB3	1.87	0.56
1:B:407:LEU:O	1:B:411:GLN:HG2	2.05	0.56
1:C:407:LEU:O	1:C:411:GLN:HG2	2.05	0.56
1:A:324:GLN:NE2	1:B:576:ARG:HD2	2.20	0.56
1:A:533:LEU:HD23	1:A:646:PHE:CD2	2.41	0.56
1:B:529:GLY:HA3	1:B:552:PHE:CZ	2.40	0.56
1:C:958:SER:C	1:C:959:LEU:HD12	2.30	0.56
1:B:676:LYS:HG3	1:B:702:PRO:HG2	1.86	0.56
1:D:974:ILE:HD11	1:D:1004:ILE:HB	1.88	0.56
1:B:551:ARG:HH22	1:B:642:THR:CG2	2.19	0.56
1:C:985:VAL:HG11	1:C:999:ARG:HD3	1.88	0.56
1:C:815:LEU:CD2	1:C:853:VAL:HG11	2.23	0.56
1:D:508:VAL:HG12	1:D:509:GLU:N	2.20	0.56
1:D:853:VAL:HG13	1:D:853:VAL:O	2.04	0.56
1:A:753:LEU:HD12	1:A:753:LEU:N	2.21	0.56
1:C:830:ARG:HG2	1:C:830:ARG:O	2.06	0.56
1:C:910:ILE:O	1:C:910:ILE:HG23	2.04	0.56
1:D:985:VAL:HG11	1:D:999:ARG:HD3	1.88	0.56
1:B:551:ARG:HH22	1:B:642:THR:HG21	1.71	0.55
1:A:407:LEU:O	1:A:411:GLN:HG2	2.05	0.55
1:A:425:TYR:OH	1:A:456:LYS:HE2	2.05	0.55
1:A:843:SER:OG	1:A:844:PRO:HD3	2.05	0.55
1:C:235:LEU:HG	1:C:236:VAL:HG23	1.88	0.55
1:D:425:TYR:OH	1:D:456:LYS:HE2	2.05	0.55
1:D:938:LYS:HE3	1:D:941:PHE:CE2	2.41	0.55
1:A:235:LEU:HG	1:A:236:VAL:HG23	1.88	0.55
1:A:830:ARG:O	1:A:830:ARG:HG2	2.06	0.55
1:C:923:ILE:HG12	1:C:924:GLY:H	1.72	0.55
1:D:533:LEU:HD13	1:D:639:SER:OG	2.05	0.55
1:D:663:LEU:HD12	1:D:792:ASP:HB3	1.75	0.55
1:D:904:ILE:HG21	1:D:907:GLU:HB2	1.88	0.55
1:A:508:VAL:O	1:A:509:GLU:HA	2.06	0.55
1:B:753:LEU:HD12	1:B:753:LEU:N	2.21	0.55
1:C:727:LEU:HD11	1:C:760:VAL:CG2	2.37	0.55
1:C:904:ILE:HG21	1:C:907:GLU:HB2	1.88	0.55
1:C:938:LYS:HE3	1:C:941:PHE:CE2	2.41	0.55
1:D:235:LEU:HG	1:D:236:VAL:HG23	1.88	0.55
1:B:830:ARG:O	1:B:830:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1015:LEU:HD21	1:C:1039:ASP:CA	2.37	0.55
1:A:727:LEU:HD11	1:A:760:VAL:CG2	2.37	0.55
1:A:938:LYS:HE3	1:A:941:PHE:CE2	2.42	0.55
1:B:727:LEU:HD11	1:B:760:VAL:CG2	2.37	0.55
1:B:808:ARG:HD2	1:B:813:LEU:C	2.32	0.55
1:C:747:VAL:HG13	1:C:747:VAL:O	2.07	0.55
1:C:753:LEU:N	1:C:753:LEU:HD12	2.21	0.55
1:D:923:ILE:HG12	1:D:924:GLY:H	1.72	0.55
1:A:808:ARG:HD2	1:A:813:LEU:C	2.32	0.55
1:C:808:ARG:HD2	1:C:813:LEU:C	2.32	0.55
1:C:894:VAL:HG21	1:C:903:PRO:HG3	1.89	0.55
1:D:1015:LEU:HD21	1:D:1039:ASP:CA	2.37	0.55
1:A:883:LEU:HD12	1:A:883:LEU:N	2.21	0.55
1:B:235:LEU:HG	1:B:236:VAL:HG23	1.88	0.55
1:B:747:VAL:O	1:B:747:VAL:HG13	2.07	0.55
1:C:873:GLY:CA	1:C:1026:ARG:HG3	2.35	0.55
1:C:883:LEU:HD12	1:C:883:LEU:N	2.22	0.55
1:C:1024:VAL:HG13	1:C:1024:VAL:O	2.06	0.55
1:B:775:SER:HB2	1:B:807:GLN:CG	2.37	0.54
1:D:747:VAL:O	1:D:747:VAL:HG13	2.07	0.54
1:D:1024:VAL:O	1:D:1024:VAL:HG13	2.06	0.54
1:B:87:PRO:HB2	1:B:109:LEU:HD11	1.90	0.54
1:C:1017:PRO:HB3	1:C:1034:GLN:CD	2.31	0.54
1:D:663:LEU:HG	1:D:792:ASP:OD2	2.08	0.54
1:D:894:VAL:HG21	1:D:903:PRO:HG3	1.89	0.54
1:D:1017:PRO:HB3	1:D:1034:GLN:CD	2.31	0.54
1:A:904:ILE:HG21	1:A:907:GLU:HB2	1.88	0.54
1:B:802:TYR:CD1	1:B:821:PHE:HD1	2.24	0.54
1:C:574:HIS:ND1	1:C:618:PRO:HD3	2.22	0.54
1:C:931:ARG:CD	1:C:942:MET:HE3	2.38	0.54
1:D:883:LEU:N	1:D:883:LEU:HD12	2.22	0.54
1:A:655:ASN:CG	1:A:658:ALA:HB2	2.32	0.54
1:B:550:ASN:CB	1:B:585:ALA:O	2.56	0.54
1:C:887:PHE:CD1	1:C:890:ILE:HD11	2.43	0.54
1:D:1020:VAL:HG23	1:D:1020:VAL:O	2.07	0.54
1:A:890:ILE:HB	1:A:893:HIS:CD2	2.42	0.54
1:C:1015:LEU:HD21	1:C:1039:ASP:CB	2.38	0.54
1:C:1020:VAL:O	1:C:1020:VAL:HG23	2.07	0.54
1:D:808:ARG:HD2	1:D:813:LEU:C	2.32	0.54
1:D:887:PHE:CD1	1:D:890:ILE:HD11	2.43	0.54
1:D:1015:LEU:HD21	1:D:1039:ASP:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:VAL:HG21	1:A:903:PRO:HG3	1.89	0.54
1:B:784:VAL:HG12	1:B:785:TRP:N	2.23	0.54
1:C:551:ARG:NH2	1:C:642:THR:HG22	2.22	0.54
1:D:574:HIS:ND1	1:D:618:PRO:HD3	2.22	0.54
1:D:775:SER:H	1:D:807:GLN:HG3	1.72	0.54
1:D:931:ARG:CD	1:D:942:MET:HE3	2.38	0.54
1:A:931:ARG:CD	1:A:942:MET:HE3	2.38	0.54
1:B:574:HIS:ND1	1:B:618:PRO:HD3	2.22	0.54
1:D:812:GLY:HA2	1:D:885:LEU:CD2	2.36	0.54
1:A:887:PHE:CD1	1:A:890:ILE:HD11	2.43	0.54
1:A:896:VAL:CG2	1:A:918:MET:HE3	2.37	0.54
1:C:774:ILE:C	1:C:806:ALA:CB	2.81	0.54
1:B:655:ASN:O	1:B:658:ALA:CB	2.56	0.54
1:B:775:SER:N	1:B:807:GLN:CD	2.50	0.54
1:D:727:LEU:HD11	1:D:760:VAL:CG2	2.37	0.54
1:D:753:LEU:HD12	1:D:753:LEU:N	2.21	0.54
1:D:784:VAL:HG12	1:D:785:TRP:N	2.23	0.54
1:D:1015:LEU:H	1:D:1015:LEU:CD1	2.21	0.54
1:A:574:HIS:ND1	1:A:618:PRO:HD3	2.22	0.54
1:C:1015:LEU:H	1:C:1015:LEU:CD1	2.21	0.54
1:A:87:PRO:HB2	1:A:109:LEU:HD11	1.90	0.53
1:A:747:VAL:HG13	1:A:747:VAL:O	2.07	0.53
1:A:907:GLU:HB3	1:A:915:VAL:HG21	1.91	0.53
1:C:784:VAL:HG12	1:C:785:TRP:N	2.23	0.53
1:C:1038:ILE:HG22	1:C:1039:ASP:N	2.23	0.53
1:D:812:GLY:HA3	1:D:885:LEU:HD21	1.84	0.53
1:D:885:LEU:HA	1:D:910:ILE:HD11	1.90	0.53
1:A:816:LYS:NZ	1:A:910:ILE:O	2.34	0.53
1:A:883:LEU:HD23	1:A:914:ILE:CD1	2.39	0.53
1:D:87:PRO:HB2	1:D:109:LEU:HD11	1.90	0.53
1:D:438:TYR:HH	1:D:527:HIS:CD2	2.23	0.53
1:D:883:LEU:HD23	1:D:914:ILE:CD1	2.39	0.53
1:D:1038:ILE:HG22	1:D:1039:ASP:N	2.23	0.53
1:A:923:ILE:HG12	1:A:924:GLY:H	1.72	0.53
1:B:550:ASN:HB2	1:B:585:ALA:O	2.09	0.53
1:B:723:LYS:N	1:B:723:LYS:HD2	2.24	0.53
1:B:533:LEU:HA	1:B:646:PHE:HB3	1.88	0.53
1:A:705:VAL:HG12	1:A:706:PRO:N	2.24	0.53
1:A:754:ARG:HG3	1:A:754:ARG:O	2.09	0.53
1:C:87:PRO:HB2	1:C:109:LEU:HD11	1.90	0.53
1:A:885:LEU:HA	1:A:910:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:GLN:C	1:C:661:LEU:HD12	2.34	0.53
1:C:876:VAL:CG2	1:C:916:CYS:HB3	2.39	0.53
1:C:883:LEU:HD23	1:C:914:ILE:CD1	2.39	0.53
1:C:988:TYR:OH	1:C:992:GLN:N	2.42	0.53
1:D:660:GLN:C	1:D:661:LEU:HD12	2.34	0.53
1:D:907:GLU:HB3	1:D:915:VAL:HG21	1.90	0.53
1:A:723:LYS:HD2	1:A:723:LYS:N	2.24	0.53
1:B:550:ASN:CG	1:B:585:ALA:O	2.46	0.53
1:B:660:GLN:C	1:B:661:LEU:HD12	2.34	0.53
1:B:802:TYR:CE2	1:B:821:PHE:CD1	2.97	0.53
1:C:712:ILE:HB	1:C:801:LEU:HD23	1.91	0.53
1:D:876:VAL:CG2	1:D:916:CYS:HB3	2.39	0.53
1:A:660:GLN:C	1:A:661:LEU:HD12	2.34	0.53
1:B:95:TYR:HA	1:B:96:PRO:C	2.33	0.53
1:B:712:ILE:HB	1:B:801:LEU:HD23	1.91	0.53
1:C:550:ASN:HB3	1:C:586:PRO:HB3	1.91	0.53
1:C:655:ASN:C	1:C:657:SER:N	2.62	0.53
1:D:988:TYR:OH	1:D:992:GLN:N	2.42	0.53
1:A:95:TYR:HA	1:A:96:PRO:C	2.33	0.52
1:A:463:PRO:CD	1:B:612:ILE:CG2	2.84	0.52
1:B:702:PRO:HA	1:B:726:ASN:HB2	1.91	0.52
1:C:907:GLU:HB3	1:C:915:VAL:HG21	1.90	0.52
1:C:885:LEU:HA	1:C:910:ILE:HD11	1.90	0.52
1:C:896:VAL:CG2	1:C:918:MET:HE3	2.37	0.52
1:C:1015:LEU:CD2	1:C:1039:ASP:HB2	2.39	0.52
1:D:443:TYR:CB	1:D:526:PRO:HB3	2.39	0.52
1:D:938:LYS:HB2	1:D:941:PHE:CD2	2.42	0.52
1:A:784:VAL:HG12	1:A:785:TRP:N	2.23	0.52
1:B:327:ASN:CG	1:B:327:ASN:O	2.52	0.52
1:D:95:TYR:HA	1:D:96:PRO:C	2.33	0.52
1:D:723:LYS:N	1:D:723:LYS:HD2	2.24	0.52
1:D:1015:LEU:CD2	1:D:1039:ASP:HB2	2.39	0.52
1:A:549:ALA:O	1:A:586:PRO:CA	2.57	0.52
1:A:816:LYS:NZ	1:A:910:ILE:HG23	2.24	0.52
1:B:533:LEU:HD21	1:B:646:PHE:CG	2.34	0.52
1:C:785:TRP:CE3	1:C:786:ASN:HB2	2.45	0.52
1:C:797:LEU:HD12	1:C:797:LEU:N	2.25	0.52
1:A:221:PHE:CZ	1:C:830:ARG:CB	2.92	0.52
1:A:785:TRP:CE3	1:A:786:ASN:HB2	2.45	0.52
1:A:797:LEU:HD12	1:A:797:LEU:N	2.25	0.52
1:C:327:ASN:CG	1:C:327:ASN:O	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:932:LEU:HD23	1:C:932:LEU:C	2.34	0.52
1:D:712:ILE:HB	1:D:801:LEU:HD23	1.91	0.52
1:A:533:LEU:CD2	1:A:646:PHE:CG	2.93	0.52
1:A:810:SER:CB	1:A:882:ASN:CG	2.71	0.52
1:A:876:VAL:CG2	1:A:916:CYS:HB3	2.39	0.52
1:A:932:LEU:HD23	1:A:932:LEU:C	2.34	0.52
1:C:723:LYS:HD2	1:C:723:LYS:N	2.24	0.52
1:C:967:SER:O	1:C:1010:PRO:HG3	2.09	0.52
1:C:1005:VAL:HG23	1:C:1005:VAL:O	2.09	0.52
1:D:785:TRP:CE3	1:D:786:ASN:HB2	2.45	0.52
1:D:996:PHE:CZ	1:D:999:ARG:HB2	2.39	0.52
1:A:890:ILE:O	1:A:893:HIS:HB3	2.09	0.52
1:B:711:LEU:HD12	1:B:711:LEU:N	2.25	0.52
1:B:797:LEU:HD12	1:B:797:LEU:N	2.25	0.52
1:B:815:LEU:CD2	1:B:853:VAL:HG11	2.23	0.52
1:C:533:LEU:HD12	1:C:642:THR:HG23	1.89	0.52
1:D:822:GLU:HG2	1:D:822:GLU:O	2.10	0.52
1:C:533:LEU:CD1	1:C:642:THR:CG2	2.83	0.52
1:C:822:GLU:HG2	1:C:822:GLU:O	2.10	0.52
1:D:967:SER:O	1:D:1010:PRO:HG3	2.09	0.52
1:C:996:PHE:CZ	1:C:999:ARG:HB2	2.39	0.52
1:A:422:LEU:HD12	1:B:605:GLN:NE2	2.25	0.52
1:B:702:PRO:O	1:B:703:GLN:HG3	2.10	0.52
1:C:988:TYR:HB3	1:C:1021:SER:O	2.09	0.52
1:D:932:LEU:C	1:D:932:LEU:HD23	2.34	0.52
1:B:754:ARG:HG3	1:B:754:ARG:O	2.09	0.51
1:C:711:LEU:HD12	1:C:711:LEU:N	2.25	0.51
1:C:754:ARG:HG3	1:C:754:ARG:O	2.09	0.51
1:D:705:VAL:HG12	1:D:706:PRO:N	2.24	0.51
1:D:711:LEU:N	1:D:711:LEU:HD12	2.25	0.51
1:D:797:LEU:HD12	1:D:797:LEU:N	2.25	0.51
1:D:890:ILE:O	1:D:893:HIS:HB3	2.10	0.51
1:D:1005:VAL:HG23	1:D:1005:VAL:O	2.09	0.51
1:A:712:ILE:HB	1:A:801:LEU:HD23	1.91	0.51
1:A:722:LEU:C	1:A:723:LYS:HD2	2.36	0.51
1:A:822:GLU:HG2	1:A:822:GLU:O	2.10	0.51
1:B:274:LEU:HD12	1:B:274:LEU:N	2.25	0.51
1:B:655:ASN:O	1:B:658:ALA:HB3	2.10	0.51
1:B:705:VAL:HG12	1:B:706:PRO:N	2.24	0.51
1:C:95:TYR:HA	1:C:96:PRO:C	2.33	0.51
1:C:993:THR:HG22	1:C:994:CYS:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:ARG:HH11	1:D:641:GLU:CD	2.16	0.51
1:D:956:VAL:O	1:D:956:VAL:HG13	2.10	0.51
1:A:327:ASN:CG	1:A:327:ASN:O	2.52	0.51
1:A:559:CYS:C	1:A:560:MET:CA	2.83	0.51
1:B:308:ARG:HB2	1:B:343:GLN:HG2	1.92	0.51
1:D:327:ASN:O	1:D:327:ASN:CG	2.52	0.51
1:D:923:ILE:HG12	1:D:924:GLY:N	2.26	0.51
1:D:988:TYR:HB3	1:D:1021:SER:O	2.09	0.51
1:A:716:GLU:HA	1:A:716:GLU:OE1	2.10	0.51
1:C:533:LEU:CD1	1:C:641:GLU:HB3	2.40	0.51
1:C:890:ILE:HB	1:C:893:HIS:CD2	2.42	0.51
1:C:956:VAL:HG13	1:C:956:VAL:O	2.10	0.51
1:D:754:ARG:HG3	1:D:754:ARG:O	2.09	0.51
1:D:993:THR:HG22	1:D:994:CYS:N	2.25	0.51
1:A:923:ILE:HG12	1:A:924:GLY:N	2.26	0.51
1:C:445:VAL:CG2	1:C:526:PRO:HG2	2.39	0.51
1:C:705:VAL:HG12	1:C:706:PRO:N	2.24	0.51
1:D:896:VAL:O	1:D:897:ALA:HB3	2.10	0.51
1:A:655:ASN:O	1:A:658:ALA:CA	2.58	0.51
1:B:785:TRP:CE3	1:B:786:ASN:HB2	2.45	0.51
1:C:533:LEU:O	1:C:644:LYS:HB2	2.10	0.51
1:C:988:TYR:C	1:C:988:TYR:CD2	2.84	0.51
1:D:574:HIS:CE1	1:D:618:PRO:HD3	2.46	0.51
1:D:713:PRO:HG3	1:D:802:TYR:CZ	2.45	0.51
1:A:176:GLU:HG3	1:A:177:GLY:N	2.26	0.51
1:A:711:LEU:N	1:A:711:LEU:HD12	2.25	0.51
1:B:235:LEU:HD21	1:B:263:PRO:HG2	1.92	0.51
1:B:470:TYR:CE1	1:B:525:ASP:OD2	2.63	0.51
1:B:676:LYS:HE2	1:B:728:PRO:CB	2.28	0.51
1:B:722:LEU:C	1:B:723:LYS:HD2	2.35	0.51
1:C:716:GLU:OE1	1:C:716:GLU:HA	2.10	0.51
1:C:954:PRO:HG3	1:C:978:TYR:O	2.10	0.51
1:D:308:ARG:HB2	1:D:343:GLN:HG2	1.92	0.51
1:D:722:LEU:C	1:D:723:LYS:HD2	2.35	0.51
1:D:954:PRO:HG3	1:D:978:TYR:O	2.10	0.51
1:A:274:LEU:HD12	1:A:274:LEU:N	2.25	0.51
1:A:574:HIS:CE1	1:A:618:PRO:HD3	2.46	0.51
1:A:816:LYS:CE	1:A:910:ILE:CG2	2.70	0.51
1:A:938:LYS:HB2	1:A:941:PHE:CD2	2.42	0.51
1:B:822:GLU:O	1:B:822:GLU:HG2	2.10	0.51
1:C:574:HIS:CE1	1:C:618:PRO:HD3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:722:LEU:C	1:C:723:LYS:HD2	2.35	0.51
1:C:871:GLU:OE1	1:C:1027:ALA:HB2	2.11	0.51
1:D:716:GLU:OE1	1:D:716:GLU:HA	2.10	0.51
1:D:799:VAL:HG23	1:D:799:VAL:O	2.11	0.51
1:A:655:ASN:C	1:A:657:SER:N	2.68	0.51
1:C:890:ILE:O	1:C:893:HIS:HB3	2.10	0.51
1:C:923:ILE:HG12	1:C:924:GLY:N	2.26	0.51
1:C:988:TYR:O	1:C:1020:VAL:HA	2.11	0.51
1:C:713:PRO:HG3	1:C:802:TYR:CZ	2.45	0.51
1:C:938:LYS:HB2	1:C:941:PHE:CD2	2.42	0.51
1:D:461:ASP:O	1:D:466:GLY:O	2.29	0.51
1:A:533:LEU:HD22	1:A:646:PHE:CD1	2.46	0.50
1:A:890:ILE:HG13	1:A:891:ALA:N	2.26	0.50
1:B:833:THR:HG23	1:B:837:HIS:HB2	1.92	0.50
1:C:461:ASP:O	1:C:466:GLY:O	2.29	0.50
1:A:713:PRO:HG3	1:A:802:TYR:CZ	2.45	0.50
1:A:833:THR:HG23	1:A:837:HIS:HB2	1.91	0.50
1:A:870:PRO:HG2	1:A:871:GLU:OE1	2.11	0.50
1:B:176:GLU:HG3	1:B:177:GLY:N	2.26	0.50
1:B:461:ASP:O	1:B:466:GLY:O	2.29	0.50
1:B:699:GLU:O	1:B:725:ARG:NH2	2.45	0.50
1:B:713:PRO:HG3	1:B:802:TYR:CZ	2.46	0.50
1:C:235:LEU:HD21	1:C:263:PRO:HG2	1.93	0.50
1:C:988:TYR:HE2	1:C:991:ASN:H	1.55	0.50
1:D:176:GLU:HG3	1:D:177:GLY:N	2.26	0.50
1:D:274:LEU:HD12	1:D:274:LEU:N	2.25	0.50
1:D:988:TYR:O	1:D:1020:VAL:HA	2.11	0.50
1:B:533:LEU:HD21	1:B:646:PHE:CZ	2.45	0.50
1:C:308:ARG:HB2	1:C:343:GLN:HG2	1.92	0.50
1:C:533:LEU:CD1	1:C:639:SER:OG	2.59	0.50
1:C:775:SER:CA	1:C:806:ALA:HB3	2.41	0.50
1:C:833:THR:HG23	1:C:837:HIS:HB2	1.92	0.50
1:D:833:THR:HG23	1:D:837:HIS:HB2	1.91	0.50
1:D:848:TRP:HA	1:D:853:VAL:HG11	1.94	0.50
1:D:896:VAL:CG2	1:D:918:MET:HE3	2.37	0.50
1:C:848:TRP:HA	1:C:853:VAL:HG11	1.94	0.50
1:C:896:VAL:O	1:C:897:ALA:HB3	2.10	0.50
1:D:470:TYR:CE1	1:D:525:ASP:CG	2.90	0.50
1:D:863:ILE:HD11	1:D:876:VAL:HB	1.94	0.50
1:D:870:PRO:HG2	1:D:871:GLU:OE1	2.11	0.50
1:A:461:ASP:O	1:A:466:GLY:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:799:VAL:HG23	1:B:799:VAL:O	2.11	0.50
1:C:988:TYR:CE2	1:C:990:GLY:N	2.80	0.50
1:D:988:TYR:CE2	1:D:990:GLY:N	2.80	0.50
1:A:308:ARG:HB2	1:A:343:GLN:HG2	1.92	0.50
1:B:574:HIS:CE1	1:B:618:PRO:HD3	2.46	0.50
1:B:716:GLU:OE1	1:B:716:GLU:HA	2.10	0.50
1:D:890:ILE:HB	1:D:893:HIS:CD2	2.42	0.50
1:A:863:ILE:HD11	1:A:876:VAL:HB	1.94	0.50
1:D:550:ASN:CB	1:D:586:PRO:CA	2.85	0.50
1:D:988:TYR:C	1:D:988:TYR:CD2	2.84	0.50
1:A:815:LEU:CA	1:A:848:TRP:CD1	2.94	0.50
1:C:274:LEU:HD12	1:C:274:LEU:N	2.25	0.50
1:C:815:LEU:CA	1:C:848:TRP:CD1	2.94	0.50
1:D:235:LEU:HD21	1:D:263:PRO:HG2	1.93	0.50
1:A:539:ARG:HD2	1:A:542:LYS:NZ	2.27	0.50
1:C:539:ARG:HD2	1:C:542:LYS:NZ	2.27	0.50
1:D:508:VAL:CG1	1:D:509:GLU:N	2.67	0.50
1:D:815:LEU:CA	1:D:848:TRP:CD1	2.94	0.50
1:A:235:LEU:HD21	1:A:263:PRO:HG2	1.92	0.49
1:B:815:LEU:CA	1:B:848:TRP:CD1	2.94	0.49
1:C:559:CYS:O	1:C:584:ASP:HB3	2.10	0.49
1:C:863:ILE:HD11	1:C:876:VAL:HB	1.93	0.49
1:C:933:CYS:HA	1:C:942:MET:SD	2.53	0.49
1:D:539:ARG:HD2	1:D:542:LYS:NZ	2.27	0.49
1:A:799:VAL:HG23	1:A:799:VAL:O	2.11	0.49
1:A:848:TRP:HA	1:A:853:VAL:HG11	1.94	0.49
1:A:933:CYS:HA	1:A:942:MET:SD	2.53	0.49
1:C:893:HIS:CE1	1:C:932:LEU:HA	2.47	0.49
1:D:775:SER:HB2	1:D:807:GLN:CB	2.42	0.49
1:A:324:GLN:NE2	1:B:576:ARG:HE	2.11	0.49
1:D:533:LEU:O	1:D:644:LYS:CG	2.61	0.49
1:D:974:ILE:CG1	1:D:1004:ILE:HB	2.43	0.49
1:D:988:TYR:HE2	1:D:991:ASN:H	1.55	0.49
1:A:673:HIS:CD2	1:A:685:PRO:HG3	2.48	0.49
1:D:984:SER:O	1:D:1024:VAL:HG23	2.13	0.49
1:B:539:ARG:HD2	1:B:542:LYS:NZ	2.27	0.49
1:C:176:GLU:HG3	1:C:177:GLY:N	2.26	0.49
1:C:673:HIS:CD2	1:C:685:PRO:HG3	2.48	0.49
1:C:799:VAL:O	1:C:799:VAL:HG23	2.11	0.49
1:C:974:ILE:CG1	1:C:1004:ILE:HB	2.43	0.49
1:D:673:HIS:CD2	1:D:685:PRO:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:898:GLY:O	1:D:900:PRO:HD3	2.12	0.49
1:D:1022:VAL:O	1:D:1022:VAL:HG13	2.12	0.49
1:A:217:LEU:CD1	1:C:940:GLU:OE1	2.55	0.49
1:A:896:VAL:O	1:A:897:ALA:HB3	2.10	0.49
1:B:705:VAL:HG13	1:B:706:PRO:HD2	1.95	0.49
1:C:677:TYR:HD1	1:C:731:GLN:CG	2.17	0.49
1:C:890:ILE:HG13	1:C:891:ALA:N	2.26	0.49
1:C:1022:VAL:HG13	1:C:1022:VAL:O	2.12	0.49
1:D:893:HIS:CE1	1:D:932:LEU:HA	2.48	0.49
1:D:970:THR:HG22	1:D:1008:SER:OG	2.13	0.49
1:A:864:LEU:HB3	1:A:877:THR:HB	1.95	0.49
1:B:237:SER:OG	1:B:238:HIS:HA	2.13	0.49
1:B:848:TRP:HA	1:B:853:VAL:HG11	1.94	0.49
1:C:137:CYS:SG	1:C:159:LEU:HD11	2.53	0.49
1:C:870:PRO:HG2	1:C:871:GLU:OE1	2.11	0.49
1:D:959:LEU:CG	1:D:974:ILE:HG22	2.28	0.49
1:A:655:ASN:CG	1:A:658:ALA:H	2.20	0.49
1:A:898:GLY:O	1:A:900:PRO:HD3	2.12	0.49
1:C:970:THR:HG22	1:C:1008:SER:OG	2.13	0.49
1:D:890:ILE:HG13	1:D:891:ALA:N	2.26	0.49
1:A:237:SER:OG	1:A:238:HIS:HA	2.13	0.49
1:A:533:LEU:CD2	1:A:646:PHE:CD1	2.96	0.49
1:B:703:GLN:O	1:B:724:ALA:HB1	2.13	0.49
1:C:984:SER:O	1:C:1024:VAL:HG23	2.13	0.49
1:C:988:TYR:CZ	1:C:991:ASN:N	2.80	0.49
1:D:988:TYR:CZ	1:D:991:ASN:N	2.80	0.49
1:A:398:VAL:HG22	1:C:946:HIS:O	2.13	0.48
1:C:560:MET:CE	1:C:586:PRO:HD3	2.43	0.48
1:C:859:GLN:OE1	1:C:859:GLN:HA	2.13	0.48
1:C:898:GLY:O	1:C:900:PRO:HD3	2.12	0.48
1:C:938:LYS:CE	1:C:941:PHE:CE2	2.96	0.48
1:C:959:LEU:CG	1:C:974:ILE:HG22	2.28	0.48
1:D:50:PHE:CE2	1:D:503:VAL:HG23	2.48	0.48
1:D:859:GLN:OE1	1:D:859:GLN:HA	2.13	0.48
1:D:864:LEU:HB3	1:D:877:THR:HB	1.95	0.48
1:D:933:CYS:HA	1:D:942:MET:SD	2.53	0.48
1:A:893:HIS:CE1	1:A:932:LEU:HA	2.48	0.48
1:B:459:ARG:HG3	1:B:526:PRO:HG3	1.94	0.48
1:C:533:LEU:CD2	1:C:639:SER:CB	2.84	0.48
1:A:411:GLN:HA	1:A:412:PRO:C	2.38	0.48
1:A:705:VAL:HG13	1:A:706:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:GLN:O	1:C:724:ALA:HB1	2.14	0.48
1:C:804:CYS:SG	1:C:833:THR:HA	2.54	0.48
1:C:864:LEU:HB3	1:C:877:THR:HB	1.95	0.48
1:D:137:CYS:SG	1:D:159:LEU:HD11	2.53	0.48
1:D:411:GLN:HA	1:D:412:PRO:C	2.38	0.48
1:D:661:LEU:HD21	1:D:790:ILE:HG13	1.94	0.48
1:D:711:LEU:HD23	1:D:821:PHE:CE1	2.48	0.48
1:D:829:GLU:O	1:D:830:ARG:HB3	2.14	0.48
1:B:137:CYS:SG	1:B:159:LEU:HD11	2.53	0.48
1:B:804:CYS:SG	1:B:833:THR:HA	2.54	0.48
1:D:703:GLN:O	1:D:724:ALA:HB1	2.14	0.48
1:D:804:CYS:SG	1:D:833:THR:HA	2.53	0.48
1:A:50:PHE:CE2	1:A:503:VAL:HG23	2.48	0.48
1:A:859:GLN:OE1	1:A:859:GLN:HA	2.13	0.48
1:B:50:PHE:CE2	1:B:503:VAL:HG23	2.48	0.48
1:B:732:SER:CB	1:D:83:HIS:NE2	2.75	0.48
1:D:440:TYR:CG	1:D:527:HIS:CD2	3.01	0.48
1:D:705:VAL:HG13	1:D:706:PRO:HD2	1.95	0.48
1:B:829:GLU:O	1:B:830:ARG:HB3	2.14	0.48
1:C:50:PHE:CE2	1:C:503:VAL:HG23	2.48	0.48
1:C:237:SER:OG	1:C:238:HIS:HA	2.13	0.48
1:C:959:LEU:HD12	1:C:1033:LEU:HD23	1.94	0.48
1:D:351:ASP:HA	1:D:431:ARG:HB2	1.96	0.48
1:D:848:TRP:HA	1:D:853:VAL:CG1	2.44	0.48
1:D:938:LYS:CE	1:D:941:PHE:CE2	2.97	0.48
1:A:221:PHE:CE1	1:C:830:ARG:HB2	2.49	0.48
1:A:938:LYS:CE	1:A:941:PHE:CE2	2.97	0.48
1:C:351:ASP:HA	1:C:431:ARG:HB2	1.96	0.48
1:C:559:CYS:O	1:C:584:ASP:HB2	2.14	0.48
1:C:705:VAL:HG13	1:C:706:PRO:HD2	1.95	0.48
1:C:932:LEU:HD23	1:C:933:CYS:N	2.28	0.48
1:A:594:CYS:O	1:A:601:GLU:HA	2.14	0.48
1:A:816:LYS:CD	1:A:910:ILE:HG23	2.44	0.48
1:C:411:GLN:HA	1:C:412:PRO:C	2.38	0.48
1:C:848:TRP:HA	1:C:853:VAL:CG1	2.44	0.48
1:D:594:CYS:O	1:D:601:GLU:HA	2.14	0.48
1:D:842:SER:HB2	1:D:844:PRO:HD2	1.96	0.48
1:D:933:CYS:SG	1:D:937:CYS:N	2.87	0.48
1:A:932:LEU:HD23	1:A:933:CYS:N	2.28	0.48
1:B:594:CYS:O	1:B:601:GLU:HA	2.14	0.48
1:B:673:HIS:CD2	1:B:685:PRO:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:960:SER:CB	1:C:973:THR:HB	2.43	0.48
1:D:237:SER:OG	1:D:238:HIS:HA	2.13	0.48
1:D:875:ARG:HG2	1:D:915:VAL:CG1	2.44	0.48
1:A:137:CYS:SG	1:A:159:LEU:HD11	2.53	0.48
1:A:848:TRP:HA	1:A:853:VAL:CG1	2.44	0.48
1:A:851:HIS:ND1	1:A:886:ASP:OD2	2.47	0.48
1:B:690:PHE:CE2	1:B:731:GLN:HG3	2.49	0.48
1:B:842:SER:HB2	1:B:844:PRO:HD2	1.96	0.48
1:B:848:TRP:HA	1:B:853:VAL:CG1	2.44	0.48
1:C:326:PHE:CG	1:C:359:PRO:HG3	2.49	0.48
1:C:933:CYS:SG	1:C:937:CYS:N	2.87	0.48
1:D:960:SER:CB	1:D:973:THR:HB	2.43	0.48
1:A:695:ILE:CD1	1:A:702:PRO:HD3	2.44	0.47
1:A:797:LEU:HD12	1:A:797:LEU:H	1.79	0.47
1:A:829:GLU:O	1:A:830:ARG:HB3	2.14	0.47
1:A:842:SER:HB2	1:A:844:PRO:HD2	1.96	0.47
1:B:797:LEU:HD12	1:B:797:LEU:H	1.79	0.47
1:C:829:GLU:O	1:C:830:ARG:HB3	2.14	0.47
1:D:812:GLY:HA2	1:D:885:LEU:HD22	1.93	0.47
1:D:833:THR:HG21	1:D:837:HIS:CB	2.44	0.47
1:A:141:ARG:HD2	1:A:143:ASP:OD1	2.14	0.47
1:A:804:CYS:SG	1:A:833:THR:HA	2.54	0.47
1:B:326:PHE:CG	1:B:359:PRO:HG3	2.49	0.47
1:D:932:LEU:HD23	1:D:933:CYS:N	2.28	0.47
1:A:326:PHE:CG	1:A:359:PRO:HG3	2.50	0.47
1:B:411:GLN:HA	1:B:412:PRO:C	2.38	0.47
1:B:470:TYR:HE1	1:B:525:ASP:OD2	1.98	0.47
1:C:594:CYS:O	1:C:601:GLU:HA	2.14	0.47
1:D:560:MET:CE	1:D:586:PRO:HD3	2.43	0.47
1:D:1022:VAL:HG13	1:D:1029:VAL:HG12	1.94	0.47
1:B:141:ARG:HD2	1:B:143:ASP:OD1	2.14	0.47
1:C:833:THR:HG21	1:C:837:HIS:CB	2.44	0.47
1:C:876:VAL:O	1:C:876:VAL:HG23	2.14	0.47
1:A:351:ASP:HA	1:A:431:ARG:HB2	1.96	0.47
1:A:695:ILE:HD13	1:A:702:PRO:HD3	1.97	0.47
1:A:903:PRO:HA	1:A:916:CYS:HA	1.96	0.47
1:C:141:ARG:HD2	1:C:143:ASP:OD1	2.14	0.47
1:C:1022:VAL:HG13	1:C:1029:VAL:HG12	1.94	0.47
1:A:713:PRO:HG3	1:A:802:TYR:HH	1.80	0.47
1:D:959:LEU:HD12	1:D:1033:LEU:HD23	1.94	0.47
1:A:655:ASN:OD1	1:A:657:SER:CA	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:GLN:O	1:A:724:ALA:HB1	2.13	0.47
1:A:833:THR:HG21	1:A:837:HIS:CB	2.44	0.47
1:A:876:VAL:O	1:A:876:VAL:HG23	2.14	0.47
1:A:933:CYS:SG	1:A:937:CYS:N	2.87	0.47
1:B:655:ASN:CA	1:B:656:CYS:N	2.69	0.47
1:B:712:ILE:HD12	1:B:799:VAL:HB	1.97	0.47
1:B:803:LYS:C	1:B:804:CYS:C	2.82	0.47
1:D:326:PHE:CG	1:D:359:PRO:HG3	2.49	0.47
1:D:534:HIS:CD2	1:D:644:LYS:HZ2	2.32	0.47
1:D:863:ILE:HG13	1:D:877:THR:C	2.40	0.47
1:A:463:PRO:O	1:B:577:LEU:HD21	2.14	0.47
1:A:663:LEU:HD11	1:A:703:GLN:HE21	1.80	0.47
1:C:797:LEU:HD12	1:C:797:LEU:H	1.79	0.47
1:C:863:ILE:HG13	1:C:877:THR:C	2.40	0.47
1:C:874:THR:HG22	1:C:875:ARG:N	2.30	0.47
1:C:875:ARG:HG2	1:C:915:VAL:CG1	2.44	0.47
1:D:701:CYS:HA	1:D:702:PRO:HD3	1.75	0.47
1:D:874:THR:HG22	1:D:875:ARG:N	2.30	0.47
1:B:833:THR:HG21	1:B:837:HIS:CB	2.44	0.47
1:C:737:TYR:HE1	1:C:754:ARG:CD	2.25	0.47
1:C:960:SER:HB2	1:C:961:PRO:CD	2.45	0.47
1:D:141:ARG:HD2	1:D:143:ASP:OD1	2.14	0.47
1:D:550:ASN:ND2	1:D:585:ALA:O	2.48	0.47
1:D:638:ARG:HB2	1:D:645:ILE:HD13	1.97	0.47
1:D:960:SER:HB2	1:D:961:PRO:CD	2.45	0.47
1:A:875:ARG:HG2	1:A:915:VAL:CG1	2.44	0.47
1:B:351:ASP:HA	1:B:431:ARG:HB2	1.96	0.47
1:C:655:ASN:O	1:C:656:CYS:C	2.54	0.47
1:D:869:PRO:HD3	1:D:981:ALA:HB1	1.97	0.47
1:B:549:ALA:C	1:B:586:PRO:HA	2.40	0.46
1:C:842:SER:HB2	1:C:844:PRO:HD2	1.96	0.46
1:A:655:ASN:CB	1:A:658:ALA:CB	2.77	0.46
1:D:159:LEU:HD13	1:D:184:ILE:HD13	1.98	0.46
1:A:476:PHE:CE2	1:A:482:ILE:HD13	2.51	0.46
1:A:663:LEU:HD11	1:A:703:GLN:NE2	2.30	0.46
1:A:712:ILE:HD12	1:A:799:VAL:HB	1.97	0.46
1:B:277:THR:HG22	1:B:279:ARG:HG3	1.98	0.46
1:C:328:ILE:HB	1:C:332:GLU:OE1	2.16	0.46
1:C:712:ILE:HD12	1:C:799:VAL:HB	1.97	0.46
1:D:775:SER:N	1:D:807:GLN:HG3	2.30	0.46
1:D:893:HIS:CG	1:D:894:VAL:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ARG:HB2	1:A:542:LYS:HD3	1.97	0.46
1:A:655:ASN:OD1	1:A:657:SER:C	2.58	0.46
1:B:638:ARG:HB2	1:B:645:ILE:HD13	1.97	0.46
1:C:159:LEU:HD13	1:C:184:ILE:HD13	1.98	0.46
1:C:875:ARG:HD3	1:C:907:GLU:OE1	2.16	0.46
1:D:445:VAL:CG2	1:D:526:PRO:HG2	2.44	0.46
1:D:712:ILE:HD12	1:D:799:VAL:HB	1.97	0.46
1:D:876:VAL:O	1:D:876:VAL:HG23	2.14	0.46
1:A:159:LEU:HD13	1:A:184:ILE:HD13	1.98	0.46
1:A:893:HIS:CG	1:A:894:VAL:N	2.83	0.46
1:B:654:TYR:CD2	1:B:670:PHE:CG	3.04	0.46
1:D:988:TYR:HE1	1:D:992:GLN:O	1.97	0.46
1:A:81:VAL:HG11	1:A:145:LEU:HB2	1.98	0.46
1:A:277:THR:HG22	1:A:279:ARG:HG3	1.98	0.46
1:A:875:ARG:HD3	1:A:907:GLU:OE1	2.16	0.46
1:B:328:ILE:HB	1:B:332:GLU:OE1	2.16	0.46
1:C:781:PHE:CD1	1:C:781:PHE:C	2.94	0.46
1:C:903:PRO:HA	1:C:916:CYS:HA	1.96	0.46
1:D:328:ILE:HB	1:D:332:GLU:OE1	2.16	0.46
1:A:328:ILE:HB	1:A:332:GLU:OE1	2.16	0.46
1:C:638:ARG:HB2	1:C:645:ILE:HD13	1.97	0.46
1:C:893:HIS:CG	1:C:894:VAL:N	2.83	0.46
1:A:781:PHE:CD1	1:A:781:PHE:C	2.94	0.46
1:A:863:ILE:HG13	1:A:877:THR:C	2.40	0.46
1:B:508:VAL:HG12	1:B:539:ARG:NH2	2.30	0.46
1:C:476:PHE:CE2	1:C:482:ILE:HD13	2.51	0.46
1:C:663:LEU:CG	1:C:792:ASP:OD2	2.59	0.46
1:C:988:TYR:HE1	1:C:992:GLN:O	1.97	0.46
1:D:476:PHE:CE2	1:D:482:ILE:HD13	2.51	0.46
1:D:903:PRO:HA	1:D:916:CYS:HA	1.96	0.46
1:D:988:TYR:CE1	1:D:992:GLN:O	2.68	0.46
1:A:654:TYR:HE1	1:A:656:CYS:SG	2.39	0.46
1:A:672:CYS:HB3	1:A:681:CYS:SG	2.56	0.46
1:A:737:TYR:CE2	1:A:785:TRP:HB3	2.51	0.46
1:C:988:TYR:CE1	1:C:992:GLN:O	2.68	0.46
1:D:875:ARG:HD3	1:D:907:GLU:OE1	2.16	0.46
1:D:979:LEU:HD12	1:D:1003:GLU:HA	1.97	0.46
1:A:112:ASN:HB2	1:A:132:LEU:HD22	1.98	0.46
1:A:550:ASN:HB2	1:A:585:ALA:O	2.16	0.46
1:B:329:SER:HB3	1:B:332:GLU:HG3	1.98	0.46
1:D:539:ARG:HB2	1:D:542:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:797:LEU:HD12	1:D:797:LEU:H	1.79	0.46
1:D:904:ILE:HG23	1:D:904:ILE:O	2.15	0.46
1:A:545:ARG:NH1	1:A:641:GLU:OE2	2.49	0.45
1:B:476:PHE:CE2	1:B:482:ILE:HD13	2.51	0.45
1:C:533:LEU:CB	1:C:642:THR:CG2	2.73	0.45
1:C:672:CYS:HB3	1:C:681:CYS:SG	2.56	0.45
1:C:785:TRP:CD1	1:C:791:ILE:HD11	2.51	0.45
1:A:463:PRO:O	1:B:614:ILE:HG12	2.14	0.45
1:A:904:ILE:HG23	1:A:904:ILE:O	2.15	0.45
1:B:539:ARG:HB2	1:B:542:LYS:HD3	1.97	0.45
1:B:737:TYR:CE2	1:B:785:TRP:HB3	2.51	0.45
1:C:979:LEU:HD12	1:C:1003:GLU:HA	1.98	0.45
1:B:112:ASN:HB2	1:B:132:LEU:HD22	1.98	0.45
1:C:112:ASN:HB2	1:C:132:LEU:HD22	1.98	0.45
1:C:539:ARG:HB2	1:C:542:LYS:HD3	1.97	0.45
1:C:737:TYR:CE2	1:C:785:TRP:HB3	2.51	0.45
1:D:979:LEU:HD12	1:D:1002:ASN:C	2.41	0.45
1:B:159:LEU:HD13	1:B:184:ILE:HD13	1.98	0.45
1:B:560:MET:CE	1:B:586:PRO:HD3	2.43	0.45
1:B:732:SER:HA	1:D:147:ILE:HD11	1.98	0.45
1:C:979:LEU:HD12	1:C:1002:ASN:C	2.41	0.45
1:D:277:THR:HG22	1:D:279:ARG:HG3	1.98	0.45
1:D:672:CYS:HB3	1:D:681:CYS:SG	2.56	0.45
1:B:81:VAL:HG11	1:B:145:LEU:HB2	1.98	0.45
1:B:672:CYS:HB3	1:B:681:CYS:SG	2.56	0.45
1:B:781:PHE:CD1	1:B:781:PHE:C	2.94	0.45
1:D:735:ARG:HG3	1:D:786:ASN:HA	1.96	0.45
1:B:534:HIS:CD2	1:B:644:LYS:HG3	2.51	0.45
1:B:690:PHE:CE2	1:B:731:GLN:HB3	2.38	0.45
1:D:785:TRP:CD1	1:D:791:ILE:HD11	2.51	0.45
1:A:874:THR:HG22	1:A:875:ARG:N	2.30	0.45
1:B:785:TRP:CD1	1:B:791:ILE:HD11	2.51	0.45
1:D:781:PHE:C	1:D:781:PHE:CD1	2.94	0.45
1:A:324:GLN:HE22	1:B:576:ARG:HA	1.82	0.45
1:B:802:TYR:CE2	1:B:821:PHE:HB3	2.51	0.45
1:D:112:ASN:HB2	1:D:132:LEU:HD22	1.98	0.45
1:D:551:ARG:HH12	1:D:641:GLU:CG	2.30	0.45
1:A:638:ARG:HB2	1:A:645:ILE:HD13	1.97	0.45
1:C:329:SER:HB3	1:C:332:GLU:HG3	1.98	0.45
1:C:808:ARG:HD2	1:C:813:LEU:O	2.17	0.45
1:C:954:PRO:HA	1:C:978:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1022:VAL:CG1	1:C:1029:VAL:CG1	2.94	0.45
1:D:1022:VAL:CG1	1:D:1029:VAL:CG1	2.94	0.45
1:A:162:VAL:CG2	1:A:189:ASP:HB2	2.47	0.45
1:A:407:LEU:HD22	1:C:944:LYS:CD	2.04	0.45
1:A:705:VAL:CG1	1:A:706:PRO:N	2.80	0.45
1:B:533:LEU:HD23	1:B:533:LEU:HA	1.84	0.45
1:C:162:VAL:CG2	1:C:189:ASP:HB2	2.47	0.45
1:C:533:LEU:HD23	1:C:533:LEU:HA	1.84	0.45
1:D:81:VAL:HG11	1:D:145:LEU:HB2	1.98	0.45
1:D:162:VAL:CG2	1:D:189:ASP:HB2	2.47	0.45
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.84	0.44
1:D:920:HIS:CD2	1:D:922:VAL:H	2.35	0.44
1:D:954:PRO:HA	1:D:978:TYR:HB2	1.99	0.44
1:A:407:LEU:CD2	1:C:944:LYS:HZ2	2.27	0.44
1:A:785:TRP:CD1	1:A:791:ILE:HD11	2.52	0.44
1:B:203:LEU:HD23	1:B:203:LEU:HA	1.84	0.44
1:C:985:VAL:O	1:C:985:VAL:HG23	2.16	0.44
1:D:737:TYR:CE2	1:D:785:TRP:HB3	2.51	0.44
1:D:985:VAL:O	1:D:985:VAL:HG23	2.16	0.44
1:A:329:SER:HB3	1:A:332:GLU:HG3	1.98	0.44
1:C:277:THR:HG22	1:C:279:ARG:HG3	1.98	0.44
1:C:904:ILE:HG23	1:C:904:ILE:O	2.15	0.44
1:C:920:HIS:CD2	1:C:922:VAL:H	2.35	0.44
1:C:992:GLN:OE1	1:C:1012:SER:HB2	2.17	0.44
1:A:920:HIS:CD2	1:A:922:VAL:H	2.35	0.44
1:B:482:ILE:HG23	1:B:497:VAL:HG13	2.00	0.44
1:B:705:VAL:CG1	1:B:706:PRO:N	2.80	0.44
1:C:81:VAL:HG11	1:C:145:LEU:HB2	1.98	0.44
1:D:661:LEU:CD2	1:D:790:ILE:HG13	2.46	0.44
1:D:705:VAL:H	1:D:724:ALA:HA	1.83	0.44
1:D:855:CYS:SG	1:D:885:LEU:CD2	2.96	0.44
1:A:325:ALA:CA	1:B:577:LEU:HD13	2.46	0.44
1:B:808:ARG:HD2	1:B:813:LEU:O	2.17	0.44
1:C:149:VAL:HG22	1:C:150:GLU:N	2.33	0.44
1:C:705:VAL:CG1	1:C:706:PRO:N	2.80	0.44
1:D:808:ARG:HD2	1:D:813:LEU:O	2.17	0.44
1:D:992:GLN:OE1	1:D:1012:SER:HB2	2.17	0.44
1:B:772:MET:HB3	1:B:806:ALA:HB1	1.98	0.44
1:C:775:SER:CB	1:C:806:ALA:H	2.30	0.44
1:D:203:LEU:HD23	1:D:203:LEU:HA	1.83	0.44
1:D:705:VAL:CG1	1:D:706:PRO:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ASN:HB2	1:A:585:ALA:C	2.43	0.44
1:A:808:ARG:HD2	1:A:813:LEU:O	2.17	0.44
1:A:890:ILE:HD13	1:A:908:TYR:CZ	2.53	0.44
1:D:1015:LEU:HD21	1:D:1039:ASP:HA	2.00	0.44
1:B:191:LYS:HD2	1:B:191:LYS:N	2.33	0.44
1:C:191:LYS:N	1:C:191:LYS:HD2	2.33	0.44
1:C:482:ILE:HG23	1:C:497:VAL:HG13	2.00	0.44
1:C:525:ASP:HA	1:C:526:PRO:HD3	1.86	0.44
1:C:534:HIS:HD2	1:C:644:LYS:NZ	2.15	0.44
1:C:890:ILE:CB	1:C:893:HIS:HD2	2.30	0.44
1:D:329:SER:HB3	1:D:332:GLU:HG3	1.98	0.44
1:A:760:VAL:CG1	1:A:761:GLN:N	2.81	0.44
1:A:944:LYS:HG3	1:A:944:LYS:O	2.18	0.44
1:B:162:VAL:CG2	1:B:189:ASP:HB2	2.48	0.44
1:B:705:VAL:H	1:B:724:ALA:HA	1.83	0.44
1:C:655:ASN:OD1	1:C:657:SER:CB	2.64	0.44
1:D:149:VAL:HG22	1:D:150:GLU:N	2.33	0.44
1:D:890:ILE:HD13	1:D:908:TYR:CZ	2.53	0.44
1:A:225:LEU:C	1:A:225:LEU:HD12	2.43	0.43
1:A:463:PRO:HB2	1:B:612:ILE:HG22	2.00	0.43
1:B:459:ARG:HG3	1:B:526:PRO:CG	2.48	0.43
1:C:959:LEU:H	1:C:1033:LEU:HD21	1.83	0.43
1:D:313:ALA:HB1	1:D:335:LEU:HD11	2.00	0.43
1:D:533:LEU:CD2	1:D:639:SER:OG	2.65	0.43
1:D:959:LEU:H	1:D:1033:LEU:HD21	1.83	0.43
1:C:775:SER:HB2	1:C:806:ALA:N	2.33	0.43
1:C:995:GLU:O	1:C:1006:CYS:HB2	2.18	0.43
1:C:1015:LEU:HD21	1:C:1039:ASP:HA	2.00	0.43
1:C:1015:LEU:CD2	1:C:1039:ASP:N	2.81	0.43
1:A:57:ARG:HG2	1:A:121:TYR:CE1	2.53	0.43
1:C:313:ALA:HB1	1:C:335:LEU:HD11	2.00	0.43
1:C:507:PRO:C	1:C:509:GLU:N	2.73	0.43
1:C:947:GLN:HG3	1:C:948:GLN:N	2.34	0.43
1:D:1015:LEU:CD2	1:D:1039:ASP:N	2.81	0.43
1:A:313:ALA:HB1	1:A:335:LEU:HD11	2.00	0.43
1:B:533:LEU:HD21	1:B:646:PHE:CD2	2.47	0.43
1:D:482:ILE:HG23	1:D:497:VAL:HG13	2.00	0.43
1:D:655:ASN:O	1:D:656:CYS:C	2.58	0.43
1:B:735:ARG:HG3	1:B:786:ASN:HA	1.95	0.43
1:C:57:ARG:HG2	1:C:121:TYR:CE1	2.53	0.43
1:C:890:ILE:HD13	1:C:908:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:944:LYS:HG3	1:C:944:LYS:O	2.18	0.43
1:C:974:ILE:O	1:C:974:ILE:HG13	2.18	0.43
1:B:741:LEU:HD12	1:B:767:TYR:CD1	2.54	0.43
1:B:802:TYR:CE1	1:B:821:PHE:CD1	3.05	0.43
1:C:56:HIS:HB3	1:C:59:THR:OG1	2.19	0.43
1:D:191:LYS:HD2	1:D:191:LYS:N	2.33	0.43
1:D:890:ILE:CB	1:D:893:HIS:HD2	2.30	0.43
1:B:533:LEU:HD21	1:B:646:PHE:CE2	2.53	0.43
1:B:568:SER:CB	1:B:670:PHE:CE1	3.02	0.43
1:B:833:THR:CG2	1:B:837:HIS:CB	2.95	0.43
1:C:225:LEU:C	1:C:225:LEU:HD12	2.43	0.43
1:C:996:PHE:HE1	1:C:1004:ILE:HG23	1.83	0.43
1:D:225:LEU:C	1:D:225:LEU:HD12	2.43	0.43
1:D:996:PHE:HE1	1:D:1004:ILE:HG23	1.83	0.43
1:A:149:VAL:HG22	1:A:150:GLU:N	2.33	0.43
1:A:191:LYS:HD2	1:A:191:LYS:N	2.33	0.43
1:D:947:GLN:HG3	1:D:948:GLN:N	2.34	0.43
1:D:974:ILE:HG13	1:D:974:ILE:O	2.18	0.43
1:D:995:GLU:O	1:D:1006:CYS:HB2	2.18	0.43
1:A:324:GLN:HE22	1:B:576:ARG:HD2	1.84	0.43
1:A:559:CYS:CA	1:A:560:MET:N	2.80	0.43
1:A:741:LEU:HD12	1:A:767:TYR:CD1	2.54	0.43
1:B:57:ARG:HG2	1:B:121:TYR:CE1	2.54	0.43
1:B:784:VAL:CG1	1:B:785:TRP:N	2.82	0.43
1:C:885:LEU:O	1:C:910:ILE:HD12	2.19	0.43
1:C:1011:SER:HB2	1:C:1037:TYR:CD1	2.54	0.43
1:D:57:ARG:HG2	1:D:121:TYR:CE1	2.54	0.43
1:D:775:SER:CA	1:D:807:GLN:HG3	2.42	0.43
1:A:560:MET:CE	1:A:586:PRO:HD3	2.43	0.43
1:A:908:TYR:CE1	1:A:914:ILE:HG12	2.54	0.43
1:B:202:LYS:C	1:B:204:PRO:HD3	2.44	0.43
1:B:690:PHE:CE2	1:B:731:GLN:CG	3.01	0.43
1:C:705:VAL:H	1:C:724:ALA:HA	1.82	0.43
1:C:741:LEU:HD12	1:C:767:TYR:CD1	2.54	0.43
1:C:908:TYR:CE1	1:C:914:ILE:HG12	2.54	0.43
1:C:987:VAL:HB	1:C:994:CYS:HB3	2.00	0.43
1:D:56:HIS:HB3	1:D:59:THR:OG1	2.19	0.43
1:D:533:LEU:HD23	1:D:533:LEU:HA	1.84	0.43
1:D:970:THR:HG22	1:D:1008:SER:CB	2.49	0.43
1:A:463:PRO:O	1:B:614:ILE:CG1	2.66	0.42
1:A:705:VAL:H	1:A:724:ALA:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:GLN:HG3	1:A:948:GLN:N	2.34	0.42
1:D:741:LEU:HD12	1:D:767:TYR:CD1	2.54	0.42
1:D:1011:SER:HB2	1:D:1037:TYR:CD1	2.54	0.42
1:A:407:LEU:HD21	1:C:944:LYS:HD3	1.77	0.42
1:A:482:ILE:HG23	1:A:497:VAL:HG13	2.00	0.42
1:A:864:LEU:CG	1:A:865:THR:N	2.82	0.42
1:B:196:PRO:HG3	1:B:215:TYR:OH	2.20	0.42
1:C:677:TYR:CE1	1:C:731:GLN:CG	3.02	0.42
1:C:848:TRP:O	1:C:848:TRP:CG	2.73	0.42
1:C:946:HIS:CG	1:C:947:GLN:N	2.87	0.42
1:C:993:THR:CG2	1:C:994:CYS:N	2.82	0.42
1:D:932:LEU:C	1:D:932:LEU:CD2	2.93	0.42
1:D:944:LYS:O	1:D:944:LYS:HG3	2.18	0.42
1:D:987:VAL:HB	1:D:994:CYS:HB3	2.00	0.42
1:D:993:THR:CG2	1:D:994:CYS:N	2.82	0.42
1:A:655:ASN:HA	1:A:656:CYS:N	2.33	0.42
1:A:784:VAL:CG1	1:A:785:TRP:N	2.82	0.42
1:A:885:LEU:O	1:A:910:ILE:HD12	2.19	0.42
1:B:149:VAL:HG22	1:B:150:GLU:N	2.33	0.42
1:C:192:GLN:HG3	1:C:228:ILE:O	2.20	0.42
1:C:970:THR:HG22	1:C:1008:SER:CB	2.49	0.42
1:D:881:VAL:CG1	1:D:882:ASN:N	2.82	0.42
1:D:1001:MET:CG	1:D:1002:ASN:N	2.83	0.42
1:A:192:GLN:HG3	1:A:228:ILE:O	2.20	0.42
1:A:810:SER:OG	1:A:882:ASN:OD1	2.37	0.42
1:A:932:LEU:C	1:A:932:LEU:CD2	2.93	0.42
1:B:225:LEU:HD12	1:B:225:LEU:C	2.43	0.42
1:B:708:GLU:HG2	1:B:709:GLU:N	2.35	0.42
1:B:760:VAL:CG1	1:B:761:GLN:N	2.81	0.42
1:C:37:GLN:OE1	1:C:37:GLN:HA	2.20	0.42
1:C:735:ARG:HG3	1:C:786:ASN:HA	1.96	0.42
1:C:931:ARG:CG	1:C:942:MET:CE	2.96	0.42
1:C:932:LEU:C	1:C:932:LEU:CD2	2.93	0.42
1:D:192:GLN:HG3	1:D:228:ILE:O	2.20	0.42
1:D:440:TYR:CD2	1:D:527:HIS:HA	2.55	0.42
1:D:482:ILE:HD12	1:D:497:VAL:HG11	2.02	0.42
1:D:706:PRO:CG	1:D:795:GLN:HG3	2.49	0.42
1:D:885:LEU:O	1:D:910:ILE:HD12	2.19	0.42
1:A:56:HIS:HB3	1:A:59:THR:OG1	2.19	0.42
1:A:704:LEU:CD1	1:A:783:VAL:HG21	2.49	0.42
1:C:482:ILE:HD12	1:C:497:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:881:VAL:CG1	1:C:882:ASN:N	2.82	0.42
1:D:37:GLN:OE1	1:D:37:GLN:HA	2.20	0.42
1:D:151:PRO:HG2	1:D:213:LEU:HD12	2.02	0.42
1:D:470:TYR:CD1	1:D:525:ASP:HB2	2.55	0.42
1:A:818:ASP:HB2	1:A:821:PHE:HD2	1.79	0.42
1:A:881:VAL:CG1	1:A:882:ASN:N	2.82	0.42
1:C:151:PRO:HG2	1:C:213:LEU:HD12	2.02	0.42
1:C:988:TYR:OH	1:C:991:ASN:N	2.53	0.42
1:C:1001:MET:CG	1:C:1002:ASN:N	2.83	0.42
1:D:1038:ILE:CG2	1:D:1039:ASP:N	2.82	0.42
1:A:324:GLN:NE2	1:B:576:ARG:NE	2.68	0.42
1:B:37:GLN:OE1	1:B:37:GLN:HA	2.20	0.42
1:B:56:HIS:HB3	1:B:59:THR:OG1	2.19	0.42
1:C:775:SER:H	1:C:807:GLN:HG3	1.85	0.42
1:C:872:GLY:O	1:C:1026:ARG:CB	2.63	0.42
1:D:202:LYS:C	1:D:204:PRO:HD3	2.44	0.42
1:D:708:GLU:HG2	1:D:709:GLU:N	2.35	0.42
1:D:908:TYR:CE1	1:D:914:ILE:HG12	2.54	0.42
1:A:202:LYS:C	1:A:204:PRO:HD3	2.44	0.42
1:A:708:GLU:HG2	1:A:709:GLU:N	2.35	0.42
1:A:815:LEU:N	1:A:815:LEU:CD1	2.83	0.42
1:C:202:LYS:C	1:C:204:PRO:HD3	2.44	0.42
1:C:708:GLU:HG2	1:C:709:GLU:N	2.35	0.42
1:C:883:LEU:HG	1:C:932:LEU:HD11	2.02	0.42
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.89	0.42
1:B:151:PRO:HG2	1:B:213:LEU:HD12	2.01	0.42
1:B:508:VAL:HG11	1:B:539:ARG:HH22	1.85	0.42
1:C:933:CYS:SG	1:C:942:MET:SD	3.18	0.42
1:C:1038:ILE:CG2	1:C:1039:ASP:N	2.82	0.42
1:D:815:LEU:N	1:D:815:LEU:CD1	2.83	0.42
1:D:933:CYS:SG	1:D:942:MET:SD	3.18	0.42
1:D:988:TYR:OH	1:D:991:ASN:N	2.53	0.42
1:A:149:VAL:HG22	1:A:151:PRO:HD3	2.02	0.42
1:A:204:PRO:HD2	1:A:212:MET:SD	2.60	0.42
1:A:848:TRP:O	1:A:848:TRP:CG	2.73	0.42
1:C:784:VAL:CG1	1:C:785:TRP:N	2.82	0.42
1:D:791:ILE:HG22	1:D:792:ASP:N	2.35	0.42
1:A:37:GLN:OE1	1:A:37:GLN:HA	2.20	0.41
1:A:196:PRO:HG3	1:A:215:TYR:OH	2.19	0.41
1:B:57:ARG:HG3	1:B:58:ARG:HG3	2.02	0.41
1:B:313:ALA:HB1	1:B:335:LEU:HD11	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:938:LYS:CE	1:C:941:PHE:HE2	2.33	0.41
1:D:784:VAL:CG1	1:D:785:TRP:N	2.82	0.41
1:D:864:LEU:CG	1:D:865:THR:N	2.82	0.41
1:D:883:LEU:HG	1:D:932:LEU:HD11	2.02	0.41
1:D:931:ARG:CG	1:D:942:MET:CE	2.96	0.41
1:B:192:GLN:HG3	1:B:228:ILE:O	2.20	0.41
1:B:476:PHE:HE2	1:B:482:ILE:HD13	1.85	0.41
1:B:482:ILE:HD12	1:B:497:VAL:HG11	2.02	0.41
1:C:716:GLU:OE2	1:C:836:GLN:HG2	2.20	0.41
1:C:833:THR:HG21	1:C:837:HIS:HB2	1.99	0.41
1:D:149:VAL:HG22	1:D:151:PRO:HD3	2.02	0.41
1:D:863:ILE:O	1:D:863:ILE:HG23	2.20	0.41
1:D:946:HIS:CG	1:D:947:GLN:N	2.87	0.41
1:D:988:TYR:OH	1:D:989:LEU:C	2.63	0.41
1:A:324:GLN:NE2	1:B:576:ARG:CD	2.84	0.41
1:A:482:ILE:HD12	1:A:497:VAL:HG11	2.02	0.41
1:A:737:TYR:HE1	1:A:754:ARG:CD	2.25	0.41
1:A:791:ILE:HG22	1:A:792:ASP:N	2.36	0.41
1:C:760:VAL:CG1	1:C:761:GLN:N	2.81	0.41
1:D:760:VAL:CG1	1:D:761:GLN:N	2.81	0.41
1:D:848:TRP:CG	1:D:848:TRP:O	2.73	0.41
1:D:931:ARG:HG2	1:D:942:MET:CE	2.50	0.41
1:A:629:ASP:OD1	1:A:659:HIS:CE1	2.72	0.41
1:A:931:ARG:CG	1:A:942:MET:CE	2.96	0.41
1:A:931:ARG:HG2	1:A:942:MET:CE	2.50	0.41
1:C:204:PRO:HD2	1:C:212:MET:SD	2.60	0.41
1:C:843:SER:N	1:C:844:PRO:CD	2.84	0.41
1:C:863:ILE:O	1:C:863:ILE:HG23	2.20	0.41
1:C:988:TYR:OH	1:C:989:LEU:C	2.63	0.41
1:C:1015:LEU:N	1:C:1015:LEU:CD1	2.83	0.41
1:D:815:LEU:O	1:D:848:TRP:CD1	2.74	0.41
1:A:815:LEU:HB3	1:A:885:LEU:CD1	2.46	0.41
1:A:883:LEU:HG	1:A:932:LEU:HD11	2.02	0.41
1:C:203:LEU:HA	1:C:203:LEU:HD23	1.83	0.41
1:C:417:THR:HA	1:C:418:PRO:HD3	1.74	0.41
1:C:815:LEU:N	1:C:815:LEU:CD1	2.83	0.41
1:D:1015:LEU:N	1:D:1015:LEU:CD1	2.83	0.41
1:A:564:VAL:HG23	1:A:649:THR:HG21	2.03	0.41
1:A:855:CYS:C	1:A:941:PHE:HE1	2.29	0.41
1:B:508:VAL:CG1	1:B:539:ARG:HH22	2.33	0.41
1:B:564:VAL:HG23	1:B:649:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:LEU:O	1:B:848:TRP:CD1	2.74	0.41
1:C:476:PHE:HE2	1:C:482:ILE:HD13	1.85	0.41
1:C:896:VAL:HG21	1:C:918:MET:CE	2.45	0.41
1:C:1018:VAL:HG12	1:C:1019:PRO:N	2.35	0.41
1:D:204:PRO:HD2	1:D:212:MET:SD	2.60	0.41
1:D:570:SER:CB	1:D:683:HIS:CG	3.03	0.41
1:D:938:LYS:CE	1:D:941:PHE:HE2	2.34	0.41
1:A:815:LEU:O	1:A:848:TRP:CD1	2.74	0.41
1:A:946:HIS:CG	1:A:947:GLN:N	2.87	0.41
1:B:204:PRO:HD2	1:B:212:MET:SD	2.60	0.41
1:B:582:VAL:CG1	1:B:585:ALA:HB2	2.51	0.41
1:B:848:TRP:O	1:B:848:TRP:CG	2.72	0.41
1:C:68:ASN:ND2	1:C:87:PRO:HG3	2.36	0.41
1:C:564:VAL:HG23	1:C:649:THR:HG21	2.03	0.41
1:D:533:LEU:CD1	1:D:641:GLU:HB3	2.51	0.41
1:D:864:LEU:CG	1:D:865:THR:H	2.32	0.41
1:A:87:PRO:HB2	1:A:109:LEU:CD1	2.51	0.41
1:A:655:ASN:CG	1:A:658:ALA:CA	2.94	0.41
1:A:843:SER:N	1:A:844:PRO:CD	2.84	0.41
1:B:843:SER:N	1:B:844:PRO:CD	2.84	0.41
1:C:864:LEU:CG	1:C:865:THR:H	2.32	0.41
1:D:68:ASN:ND2	1:D:87:PRO:HG3	2.36	0.41
1:D:196:PRO:HG3	1:D:215:TYR:OH	2.19	0.41
1:D:843:SER:N	1:D:844:PRO:CD	2.84	0.41
1:A:68:ASN:ND2	1:A:87:PRO:HG3	2.36	0.41
1:A:463:PRO:CG	1:B:612:ILE:CB	2.68	0.41
1:A:532:ALA:O	1:A:646:PHE:HB2	2.20	0.41
1:A:714:VAL:CG1	1:A:768:GLN:HA	2.49	0.41
1:A:781:PHE:CE2	1:A:797:LEU:O	2.74	0.41
1:A:933:CYS:SG	1:A:942:MET:SD	3.18	0.41
1:B:404:PHE:CE2	1:B:406:GLY:HA2	2.56	0.41
1:C:149:VAL:HG22	1:C:151:PRO:HD3	2.03	0.41
1:C:196:PRO:HG3	1:C:215:TYR:OH	2.20	0.41
1:C:315:LEU:HD11	1:C:333:ASP:HB3	2.03	0.41
1:C:709:GLU:OE1	1:C:709:GLU:HA	2.21	0.41
1:C:791:ILE:HG22	1:C:792:ASP:N	2.36	0.41
1:C:988:TYR:CZ	1:C:991:ASN:C	2.99	0.41
1:C:988:TYR:CE1	1:C:992:GLN:C	2.90	0.41
1:D:404:PHE:CE2	1:D:406:GLY:HA2	2.56	0.41
1:D:476:PHE:HE2	1:D:482:ILE:HD13	1.85	0.41
1:D:533:LEU:HD11	1:D:641:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:709:GLU:O	1:D:711:LEU:HD12	2.21	0.41
1:D:781:PHE:CE2	1:D:797:LEU:O	2.74	0.41
1:D:988:TYR:CZ	1:D:991:ASN:C	2.99	0.41
1:D:1011:SER:C	1:D:1013:ASN:N	2.77	0.41
1:D:1018:VAL:HG12	1:D:1019:PRO:N	2.35	0.41
1:A:57:ARG:HG3	1:A:58:ARG:HG3	2.02	0.41
1:A:582:VAL:CG1	1:A:585:ALA:HB2	2.51	0.41
1:A:709:GLU:O	1:A:711:LEU:HD12	2.21	0.41
1:A:883:LEU:HD13	1:A:911:ALA:O	2.21	0.41
1:B:68:ASN:ND2	1:B:87:PRO:HG3	2.36	0.41
1:B:781:PHE:CE2	1:B:797:LEU:O	2.74	0.41
1:C:815:LEU:O	1:C:848:TRP:CD1	2.74	0.41
1:C:931:ARG:HG2	1:C:942:MET:CE	2.50	0.41
1:D:309:LEU:HD23	1:D:309:LEU:HA	1.89	0.41
1:D:807:GLN:HE21	1:D:807:GLN:HB3	1.65	0.41
1:A:151:PRO:HG2	1:A:213:LEU:HD12	2.02	0.40
1:A:709:GLU:OE1	1:A:709:GLU:HA	2.21	0.40
1:B:709:GLU:O	1:B:711:LEU:HD12	2.21	0.40
1:B:815:LEU:HD23	1:B:848:TRP:HB3	2.04	0.40
1:B:815:LEU:N	1:B:815:LEU:CD1	2.83	0.40
1:C:709:GLU:O	1:C:711:LEU:HD12	2.21	0.40
1:C:864:LEU:CG	1:C:865:THR:N	2.82	0.40
1:D:564:VAL:HG23	1:D:649:THR:HG21	2.03	0.40
1:D:582:VAL:CG1	1:D:585:ALA:HB2	2.51	0.40
1:D:619:LYS:HD3	1:D:619:LYS:HA	1.91	0.40
1:A:404:PHE:CE2	1:A:406:GLY:HA2	2.56	0.40
1:A:407:LEU:HD22	1:C:944:LYS:CG	2.48	0.40
1:A:463:PRO:HD2	1:B:612:ILE:HG21	2.03	0.40
1:A:863:ILE:O	1:A:863:ILE:HG23	2.20	0.40
1:B:257:THR:O	1:B:278:SER:HA	2.22	0.40
1:C:404:PHE:CE2	1:C:406:GLY:HA2	2.56	0.40
1:C:883:LEU:HD13	1:C:911:ALA:O	2.21	0.40
1:D:633:LEU:C	1:D:633:LEU:HD12	2.46	0.40
1:A:550:ASN:O	1:A:586:PRO:HG3	2.21	0.40
1:A:633:LEU:HD12	1:A:633:LEU:C	2.46	0.40
1:A:815:LEU:HD23	1:A:848:TRP:HB3	2.04	0.40
1:A:864:LEU:CG	1:A:865:THR:H	2.32	0.40
1:A:923:ILE:CG1	1:A:924:GLY:H	2.35	0.40
1:C:702:PRO:HB3	1:C:728:PRO:CG	2.52	0.40
1:C:781:PHE:CE2	1:C:797:LEU:O	2.74	0.40
1:C:952:VAL:HG23	1:C:954:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1011:SER:C	1:C:1013:ASN:N	2.77	0.40
1:D:315:LEU:HD11	1:D:333:ASP:HB3	2.03	0.40
1:B:149:VAL:HG22	1:B:151:PRO:HD3	2.02	0.40
1:B:633:LEU:C	1:B:633:LEU:HD12	2.46	0.40
1:D:57:ARG:HG3	1:D:58:ARG:HG3	2.02	0.40
1:D:87:PRO:HB2	1:D:109:LEU:CD1	2.51	0.40
1:D:993:THR:HG22	1:D:994:CYS:O	2.22	0.40
1:A:810:SER:HB3	1:A:882:ASN:HD21	1.83	0.40
1:C:349:PRO:HA	1:C:350:PRO:HD3	1.96	0.40
1:C:979:LEU:HB2	1:C:1000:SER:O	2.21	0.40
1:C:1013:ASN:HB3	1:C:1014:GLY:H	1.68	0.40
1:D:883:LEU:HD13	1:D:911:ALA:O	2.21	0.40

All (13) 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:839:PRO:CB	1:B:768:GLN:OE1[5_665]	1.27	0.93
1:B:397:PRO:CG	1:D:947:GLN:OE1[2_564]	1.51	0.69
1:A:731:GLN:OE1	1:C:146:PHE:CD1[3_455]	1.56	0.64
1:B:407:LEU:CD2	1:D:944:LYS:CD[2_564]	1.79	0.41
1:A:731:GLN:NE2	1:C:146:PHE:CE1[3_455]	1.87	0.33
1:A:766:SER:OG	1:B:839:PRO:CA[5_665]	1.98	0.22
1:A:839:PRO:CG	1:B:768:GLN:OE1[5_665]	2.02	0.18
1:B:146:PHE:CE1	1:C:677:TYR:OH[4_565]	2.03	0.17
1:A:731:GLN:CD	1:C:146:PHE:CD1[3_455]	2.08	0.12
1:A:766:SER:OG	1:B:839:PRO:CB[5_665]	2.12	0.08
1:A:84:LYS:CB	1:D:732:SER:OG[5_555]	2.15	0.05
1:A:731:GLN:CD	1:C:146:PHE:CE1[3_455]	2.15	0.05
1:B:217:LEU:CD1	1:D:940:GLU:OE1[2_564]	2.16	0.04

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	896/1212 (74%)	861 (96%)	26 (3%)	9 (1%)	12	49
1	B	797/1212 (66%)	771 (97%)	19 (2%)	7 (1%)	14	51
1	C	981/1212 (81%)	937 (96%)	35 (4%)	9 (1%)	14	51
1	D	983/1212 (81%)	942 (96%)	31 (3%)	10 (1%)	12	49
All	All	3657/4848 (75%)	3511 (96%)	111 (3%)	35 (1%)	12	49

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	702	PRO
1	A	851	HIS
1	B	508	VAL
1	B	509	GLU
1	B	851	HIS
1	C	804	CYS
1	C	851	HIS
1	D	804	CYS
1	D	851	HIS
1	A	703	GLN
1	A	160	SER
1	A	175	SER
1	A	805	ALA
1	B	160	SER
1	B	175	SER
1	B	805	ALA
1	C	160	SER
1	C	175	SER
1	C	805	ALA
1	D	160	SER
1	D	175	SER
1	D	805	ALA
1	A	849	SER
1	B	849	SER
1	C	849	SER
1	D	559	CYS
1	D	849	SER
1	A	935	GLY
1	C	935	GLY
1	C	952	VAL
1	D	935	GLY

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Mol	Chain	Res	Type
1	D	952	VAL
1	A	922	VAL
1	C	922	VAL
1	D	922	VAL

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	796/1064 (75%)	781 (98%)	15 (2%)	50	67
1	B	714/1064 (67%)	701 (98%)	13 (2%)	51	68
1	C	870/1064 (82%)	855 (98%)	15 (2%)	53	69
1	D	870/1064 (82%)	855 (98%)	15 (2%)	53	69
All	All	3250/4256 (76%)	3192 (98%)	58 (2%)	51	68

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	VAL
1	A	237	SER
1	A	238	HIS
1	A	274	LEU
1	A	298	PHE
1	A	301	THR
1	A	508	VAL
1	A	509	GLU
1	A	512	GLU
1	A	542	LYS
1	A	580	LEU
1	A	626	LEU
1	A	811	CYS
1	A	893	HIS
1	A	932	LEU
1	B	106	VAL
1	B	237	SER

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Mol	Chain	Res	Type
1	B	238	HIS
1	B	274	LEU
1	B	298	PHE
1	B	301	THR
1	B	508	VAL
1	B	509	GLU
1	B	512	GLU
1	B	542	LYS
1	B	580	LEU
1	B	626	LEU
1	B	811	CYS
1	C	106	VAL
1	C	237	SER
1	C	238	HIS
1	C	274	LEU
1	C	298	PHE
1	C	301	THR
1	C	508	VAL
1	C	509	GLU
1	C	512	GLU
1	C	542	LYS
1	C	580	LEU
1	C	626	LEU
1	C	811	CYS
1	C	893	HIS
1	C	932	LEU
1	D	106	VAL
1	D	237	SER
1	D	238	HIS
1	D	274	LEU
1	D	298	PHE
1	D	301	THR
1	D	508	VAL
1	D	509	GLU
1	D	512	GLU
1	D	542	LYS
1	D	580	LEU
1	D	626	LEU
1	D	811	CYS
1	D	893	HIS
1	D	932	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	153	HIS
1	A	324	GLN
1	A	392	GLN
1	A	403	ASN
1	A	696	ASN
1	A	726	ASN
1	A	761	GLN
1	A	836	GLN
1	A	837	HIS
1	B	403	ASN
1	B	465	HIS
1	B	527	HIS
1	B	534	HIS
1	B	703	GLN
1	B	761	GLN
1	B	837	HIS
1	B	851	HIS
1	C	403	ASN
1	C	465	HIS
1	C	534	HIS
1	C	726	ASN
1	C	761	GLN
1	C	800	HIS
1	C	807	GLN
1	C	837	HIS
1	C	953	ASN
1	C	991	ASN
1	C	1034	GLN
1	D	403	ASN
1	D	465	HIS
1	D	534	HIS
1	D	550	ASN
1	D	726	ASN
1	D	761	GLN
1	D	807	GLN
1	D	836	GLN
1	D	837	HIS
1	D	953	ASN
1	D	991	ASN
1	D	1034	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	6
1	B	6
1	A	6
1	D	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	855:CYS	C	856:SER	N	5.61
1	C	702:PRO	C	703:GLN	N	3.75
1	D	702:PRO	C	703:GLN	N	3.35
1	C	559:CYS	C	560:MET	N	2.82
1	C	855:CYS	C	856:SER	N	2.48
1	B	559:CYS	C	560:MET	N	2.40
1	B	701:CYS	C	702:PRO	N	2.35
1	B	803:LYS	C	804:CYS	N	2.12

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	559:CYS	C	560:MET	N	2.11
1	A	655:ASN	C	656:CYS	N	2.03
1	B	702:PRO	C	703:GLN	N	1.94
1	A	702:PRO	C	703:GLN	N	1.89
1	B	655:ASN	C	656:CYS	N	1.71
1	D	952:VAL	C	953:ASN	N	1.66
1	C	701:CYS	C	702:PRO	N	1.60
1	C	803:LYS	C	804:CYS	N	1.20
1	A	701:CYS	C	702:PRO	N	1.19
1	A	803:LYS	C	804:CYS	N	1.18
1	C	508:VAL	C	509:GLU	N	1.07
1	B	508:VAL	C	509:GLU	N	0.99
1	D	508:VAL	C	509:GLU	N	0.98
1	D	655:ASN	C	656:CYS	N	0.96
1	A	508:VAL	C	509:GLU	N	0.78

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	906/1212 (74%)	0.07	54 (5%)	27	32	153, 176, 433, 433	0
1	B	809/1212 (66%)	-0.06	30 (3%)	45	43	147, 209, 350, 350	0
1	C	993/1212 (81%)	-0.17	44 (4%)	39	39	200, 270, 340, 340	0
1	D	993/1212 (81%)	-0.20	31 (3%)	51	46	184, 270, 345, 345	0
All	All	3701/4848 (76%)	-0.09	159 (4%)	40	40	147, 228, 345, 433	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	770	ASP	6.3
1	A	771	GLY	6.3
1	D	485	ASP	6.3
1	C	294	VAL	5.7
1	A	769	TYR	5.6
1	A	463	PRO	5.6
1	A	773	ASP	5.6
1	B	106	VAL	5.5
1	A	864	LEU	5.5
1	D	851	HIS	5.3
1	A	947	GLN	5.2
1	A	557	SER	5.0
1	A	746	ALA	5.0
1	A	747	VAL	5.0
1	A	875	ARG	4.9
1	C	604	GLY	4.9
1	A	745	GLY	4.9
1	D	850	SER	4.7
1	B	623	VAL	4.6
1	B	790	ILE	4.3
1	A	578	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	924	GLY	4.2
1	A	862	GLU	4.2
1	B	723	LYS	4.1
1	B	557	SER	4.1
1	C	240	ASP	4.1
1	A	866	VAL	4.0
1	A	744	GLN	4.0
1	B	794	PRO	4.0
1	C	238	HIS	4.0
1	A	462	GLY	4.0
1	B	610	GLN	3.9
1	A	522	SER	3.9
1	D	486	MET	3.8
1	D	104	SER	3.8
1	B	364	ASN	3.8
1	B	782	ALA	3.7
1	A	587	ASN	3.7
1	C	923	ILE	3.7
1	D	692	GLU	3.7
1	C	280	ILE	3.6
1	A	707	THR	3.6
1	D	460	ALA	3.5
1	A	361	ARG	3.5
1	D	778	ALA	3.5
1	A	415	GLY	3.4
1	B	595	ALA	3.3
1	B	108	THR	3.3
1	A	926	THR	3.3
1	A	594	CYS	3.3
1	D	63	TYR	3.3
1	A	577	LEU	3.2
1	D	64	VAL	3.1
1	A	863	ILE	3.1
1	A	281	VAL	3.1
1	C	581	VAL	3.1
1	C	485	ASP	3.0
1	C	397	PRO	3.0
1	B	251	GLY	3.0
1	C	987	VAL	3.0
1	D	55	VAL	3.0
1	A	37	GLN	3.0
1	B	253	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	893	HIS	2.9
1	C	257	THR	2.9
1	A	743	ILE	2.9
1	A	869	PRO	2.9
1	A	609	SER	2.9
1	D	1036	GLU	2.9
1	C	920	HIS	2.8
1	C	971	MET	2.8
1	B	721	THR	2.8
1	C	621	VAL	2.8
1	B	37	GLN	2.8
1	B	416	SER	2.8
1	A	638	ARG	2.7
1	C	304	GLY	2.7
1	C	905	PRO	2.7
1	A	772	MET	2.7
1	A	852	ASN	2.7
1	D	905	PRO	2.7
1	B	107	LEU	2.7
1	A	555	SER	2.7
1	D	798	LYS	2.7
1	C	862	GLU	2.7
1	C	460	ALA	2.6
1	D	303	ALA	2.6
1	D	331	ASP	2.6
1	A	210	SER	2.6
1	B	176	GLU	2.6
1	A	595	ALA	2.6
1	B	795	GLN	2.6
1	C	438	TYR	2.6
1	C	924	GLY	2.6
1	D	54	THR	2.6
1	B	855	CYS	2.5
1	D	119	ILE	2.5
1	A	246	GLY	2.5
1	C	613	CYS	2.4
1	A	927	SER	2.4
1	D	71	TYR	2.4
1	B	783	VAL	2.4
1	D	83	HIS	2.4
1	A	950	THR	2.4
1	C	557	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	969	GLY	2.4
1	C	583	ASN	2.4
1	D	257	THR	2.4
1	D	800	HIS	2.4
1	C	170	GLY	2.3
1	C	82	ALA	2.3
1	C	256	LEU	2.3
1	C	859	GLN	2.3
1	B	707	THR	2.3
1	B	83	HIS	2.3
1	C	312	ALA	2.3
1	A	611	VAL	2.3
1	C	605	GLN	2.3
1	C	660	GLN	2.3
1	C	947	GLN	2.3
1	B	447	PHE	2.3
1	C	798	LYS	2.3
1	B	612	ILE	2.3
1	C	303	ALA	2.2
1	C	922	VAL	2.2
1	A	830	ARG	2.2
1	A	933	CYS	2.2
1	C	861	THR	2.2
1	A	596	PHE	2.2
1	A	183	PHE	2.2
1	D	483	LEU	2.2
1	D	36	PRO	2.2
1	C	434	SER	2.2
1	A	92	LYS	2.2
1	C	458	ILE	2.2
1	A	679	ASN	2.2
1	A	397	PRO	2.1
1	A	669	ALA	2.1
1	C	986	ALA	2.1
1	C	395	LYS	2.1
1	C	946	HIS	2.1
1	D	623	VAL	2.1
1	C	281	VAL	2.1
1	D	82	ALA	2.1
1	C	622	PRO	2.1
1	D	458	ILE	2.1
1	A	708	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	474	SER	2.1
1	A	623	VAL	2.1
1	C	623	VAL	2.1
1	B	793	ASN	2.1
1	D	237	SER	2.1
1	B	636	GLN	2.0
1	A	106	VAL	2.0
1	B	221	PHE	2.0
1	A	163	ASN	2.0
1	C	603	GLU	2.0
1	B	238	HIS	2.0
1	D	777	LEU	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 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.