



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:54 AM UTC

PDB ID : 1YGU / pdb_00001ygu
Title : Crystal structure of the tandem phosphatase domains of RPTP CD45 with a pTyr peptide
Authors : Nam, H.; Poy, F.; Saito, H.; Frederick, C.A.
Deposited on : 2005-01-05
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

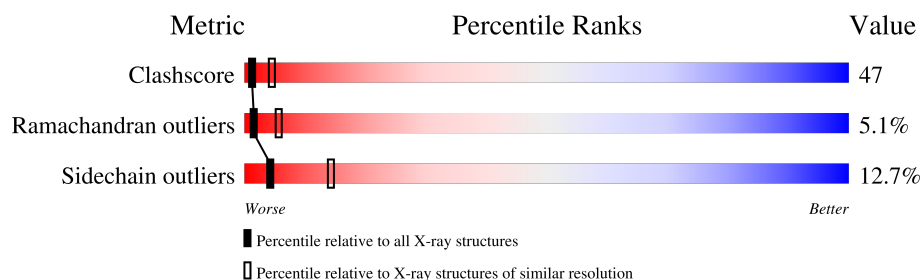
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	610	
1	B	610	
2	C	4	
2	D	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTR	C	2004	X	-	-	-
2	PTR	D	2004	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9529 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 Leukocyte common antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	Se	0	0	0
			4684	2983	815	866	7	13			
1	B	582	Total	C	N	O	S	Se	0	0	0
			4771	3033	835	883	7	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	MSE	MET	modified residue	UNP P08575
A	627	PRO	LEU	variant	UNP P08575
A	714	MSE	MET	modified residue	UNP P08575
A	725	MSE	MET	modified residue	UNP P08575
A	744	MSE	MET	modified residue	UNP P08575
A	828	SER	CYS	engineered mutation	UNP P08575
A	844	MSE	MET	modified residue	UNP P08575
A	870	MSE	MET	modified residue	UNP P08575
A	907	MSE	MET	modified residue	UNP P08575
A	999	MSE	MET	modified residue	UNP P08575
A	1007	MSE	MET	modified residue	UNP P08575
A	1024	MSE	MET	modified residue	UNP P08575
A	1035	MSE	MET	modified residue	UNP P08575
A	1115	MSE	MET	modified residue	UNP P08575
A	1184	LEU	PRO	variant	UNP P08575
A	1186	MSE	MET	modified residue	UNP P08575
B	603	MSE	MET	modified residue	UNP P08575
B	627	PRO	LEU	variant	UNP P08575
B	714	MSE	MET	modified residue	UNP P08575
B	725	MSE	MET	modified residue	UNP P08575
B	744	MSE	MET	modified residue	UNP P08575
B	828	SER	CYS	engineered mutation	UNP P08575
B	844	MSE	MET	modified residue	UNP P08575
B	870	MSE	MET	modified residue	UNP P08575
B	907	MSE	MET	modified residue	UNP P08575

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Chain	Residue	Modelled	Actual	Comment	Reference
B	999	MSE	MET	modified residue	UNP P08575
B	1007	MSE	MET	modified residue	UNP P08575
B	1024	MSE	MET	modified residue	UNP P08575
B	1035	MSE	MET	modified residue	UNP P08575
B	1115	MSE	MET	modified residue	UNP P08575
B	1184	LEU	PRO	variant	UNP P08575
B	1186	MSE	MET	modified residue	UNP P08575

- Molecule 2 is a protein called Polyoma Middle T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	P	0	0	0
			37	21	4	11	1			
2	D	4	Total	C	N	O	P	0	0	0
			37	21	4	11	1			

There are 2 discrepancies between the modelled and reference sequences:

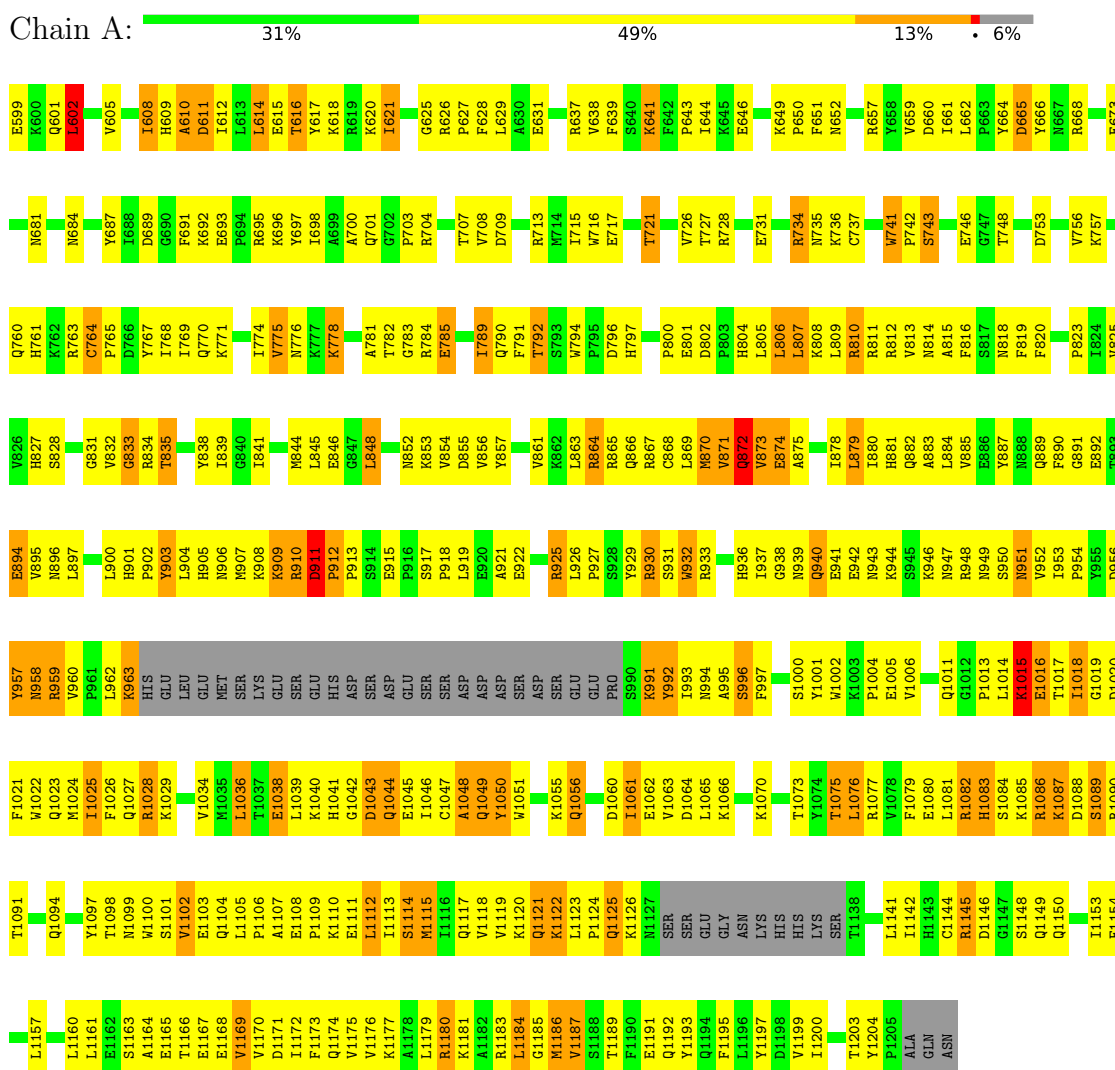
Chain	Residue	Modelled	Actual	Comment	Reference
C	2004	PTR	TYR	modified residue	UNP P03077
D	2004	PTR	TYR	modified residue	UNP P03077

3 Residue-property plots

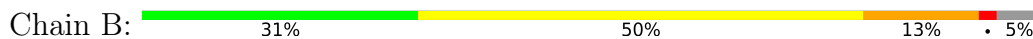
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

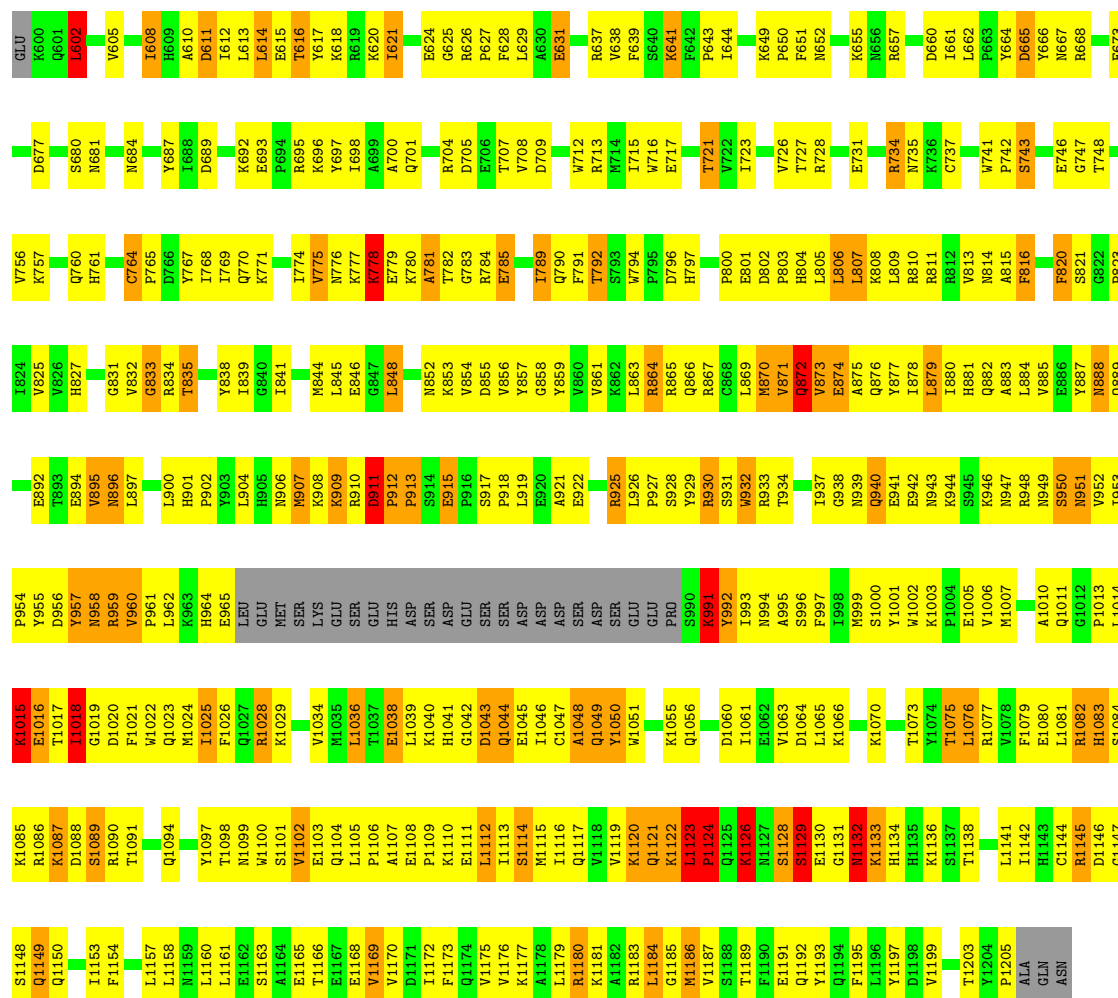
Note EDS was not executed.

- Molecule 1: Leukocyte common antigen



- Molecule 1: Leukocyte common antigen





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.90Å 57.92Å 159.29Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	29.16 – 2.90	Depositor
% Data completeness (in resolution range)	92.9 (29.16-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9529	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/4779	1.09	27/6440 (0.4%)
1	B	0.60	0/4870	1.10	38/6562 (0.6%)
2	C	0.76	0/20	1.33	0/23
2	D	0.76	0/20	1.31	0/23
All	All	0.61	0/9689	1.10	65/13048 (0.5%)

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
2	C	1	0
2	D	1	0
All	All	2	0

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	778	LYS	N-CA-C	-8.98	100.04	112.25
1	B	846	GLU	N-CA-C	-8.34	102.13	111.14
1	B	602	LEU	N-CA-C	-8.19	96.99	110.17
1	B	778	LYS	N-CA-C	-8.17	100.70	111.24
1	B	781	ALA	N-CA-C	8.11	122.64	110.64
1	A	846	GLU	N-CA-C	-8.09	102.40	111.14
1	B	960	VAL	N-CA-C	8.08	114.91	107.56
1	A	872	GLN	N-CA-C	7.83	122.46	113.15
1	A	781	ALA	N-CA-C	-7.77	97.25	109.07
1	A	602	LEU	N-CA-C	-7.55	101.50	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1112	LEU	N-CA-C	-7.51	103.11	111.82
1	B	764	CYS	CA-C-N	7.15	127.47	119.32
1	B	764	CYS	C-N-CA	7.15	127.47	119.32
1	A	894	GLU	N-CA-C	7.13	121.14	108.24
1	A	911	ASP	CA-C-N	-7.12	113.05	120.38
1	A	911	ASP	C-N-CA	-7.12	113.05	120.38
1	A	1125	GLN	N-CA-C	7.09	120.52	109.96
1	A	992	TYR	N-CA-C	7.02	120.69	109.24
1	B	872	GLN	N-CA-C	6.85	121.25	113.02
1	B	1124	PRO	N-CA-C	6.79	126.47	112.47
1	A	1112	LEU	N-CA-C	-6.73	104.02	111.82
1	B	1126	LYS	N-CA-C	6.69	119.11	109.14
1	B	616	THR	N-CA-C	-6.66	103.12	111.11
1	B	666	TYR	N-CA-C	6.62	118.58	111.36
1	A	764	CYS	CA-C-N	6.58	126.83	119.32
1	A	764	CYS	C-N-CA	6.58	126.83	119.32
1	B	1123	LEU	N-CA-C	6.50	124.17	109.81
1	A	666	TYR	N-CA-C	6.48	118.42	111.36
1	A	912	PRO	N-CA-C	-6.43	102.85	110.70
1	B	807	LEU	N-CA-C	-6.38	105.22	112.87
1	A	1126	LYS	N-CA-C	6.36	124.34	110.80
1	A	810	ARG	N-CA-C	-6.26	104.53	111.36
1	B	1129	SER	N-CA-C	-6.13	97.75	110.80
1	B	950	SER	N-CA-C	5.96	118.29	111.02
1	B	608	ILE	N-CA-C	5.87	117.29	109.37
1	A	807	LEU	N-CA-C	-5.73	105.99	112.87
1	A	743	SER	N-CA-C	-5.70	102.61	110.35
1	B	705	ASP	N-CA-C	-5.64	105.13	111.28
1	B	907	MSE	N-CA-C	-5.58	106.18	112.87
1	B	959	ARG	CA-C-N	-5.56	118.82	122.60
1	B	959	ARG	C-N-CA	-5.56	118.82	122.60
1	B	816	PHE	N-CA-C	5.46	117.92	110.55
1	B	1123	LEU	CA-C-N	5.45	126.65	119.84
1	B	1123	LEU	C-N-CA	5.45	126.65	119.84
1	B	821	SER	N-CA-C	-5.45	104.39	111.74
1	B	1080	GLU	N-CA-C	-5.41	99.47	108.34
1	A	616	THR	N-CA-C	-5.41	102.45	111.37
1	A	1080	GLU	N-CA-C	-5.38	99.67	108.76
1	B	743	SER	N-CA-C	-5.35	103.07	110.35
1	B	873	VAL	N-CA-C	5.35	115.60	108.27
1	B	1038	GLU	N-CA-C	-5.32	101.59	109.94
1	A	873	VAL	N-CA-C	5.31	115.54	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	608	ILE	N-CA-C	5.25	116.45	109.37
1	A	1038	GLU	N-CA-C	-5.25	101.70	109.94
1	B	1124	PRO	CA-C-N	5.24	131.54	121.54
1	B	1124	PRO	C-N-CA	5.24	131.54	121.54
1	B	912	PRO	CA-C-N	5.22	126.37	119.84
1	B	912	PRO	C-N-CA	5.22	126.37	119.84
1	B	912	PRO	N-CA-C	-5.20	104.36	110.70
1	B	911	ASP	CA-C-N	-5.08	115.15	120.38
1	B	911	ASP	C-N-CA	-5.08	115.15	120.38
1	A	741	TRP	CA-C-N	5.07	125.22	119.90
1	A	741	TRP	C-N-CA	5.07	125.22	119.90
1	A	868	CYS	N-CA-C	5.03	117.76	110.42
1	B	631	GLU	N-CA-C	-5.01	105.26	111.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2004	PTR	CA
2	D	2004	PTR	CA

There are no planarity outliers.

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	4684	0	4645	430	0
1	B	4771	0	4723	461	0
2	C	37	0	25	1	0
2	D	37	0	25	1	0
All	All	9529	0	9418	892	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (892) 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:1179:LEU:HD22	1:A:1186:MSE:HE3	1.27	1.14
1:A:874:GLU:CD	1:A:874:GLU:H	1.50	1.13
1:B:844:MSE:HE3	1:B:854:VAL:HB	1.28	1.11
1:A:844:MSE:HE3	1:A:854:VAL:HB	1.34	1.08
1:B:874:GLU:CD	1:B:874:GLU:H	1.61	1.08
1:B:912:PRO:HB2	1:B:915:GLU:HG2	1.35	1.05
1:A:911:ASP:HB3	1:A:912:PRO:HD3	1.39	1.00
1:A:1153:ILE:HD11	1:A:1192:GLN:HB3	1.46	0.98
1:B:911:ASP:HB2	1:B:912:PRO:HD3	1.48	0.93
1:B:962:LEU:HB3	1:B:991:LYS:HZ3	1.34	0.93
1:B:784:ARG:HD2	1:B:820:PHE:CZ	2.03	0.92
1:A:1040:LYS:HB3	1:A:1045:GLU:HA	1.51	0.91
1:B:1040:LYS:HB3	1:B:1045:GLU:HA	1.50	0.91
1:B:895:VAL:HG22	1:B:896:ASN:H	1.36	0.91
1:A:761:HIS:HD2	1:A:770:GLN:HE21	1.19	0.91
1:A:602:LEU:HD22	1:A:602:LEU:H	1.37	0.89
1:B:813:VAL:HG21	1:B:838:TYR:OH	1.73	0.89
1:B:1153:ILE:HD11	1:B:1192:GLN:HB3	1.51	0.89
1:B:844:MSE:CE	1:B:854:VAL:HB	2.01	0.89
1:A:873:VAL:HG12	1:A:875:ALA:H	1.40	0.86
1:B:1083:HIS:CE1	1:B:1085:LYS:HE2	2.10	0.86
1:B:1044:GLN:H	1:B:1044:GLN:NE2	1.74	0.86
1:B:785:GLU:H	1:B:785:GLU:CD	1.81	0.85
1:A:1115:MSE:O	1:A:1119:VAL:HG23	1.76	0.85
1:B:605:VAL:HG21	1:B:857:TYR:HB3	1.58	0.85
1:A:1179:LEU:HD22	1:A:1186:MSE:CE	2.06	0.84
1:B:777:LYS:NZ	1:B:781:ALA:HB3	1.93	0.83
1:A:813:VAL:HG21	1:A:838:TYR:OH	1.78	0.83
1:A:1022:TRP:HE1	1:A:1050:TYR:HB2	1.43	0.83
1:B:910:ARG:HD3	1:B:915:GLU:O	1.77	0.83
1:A:809:LEU:O	1:A:813:VAL:HG22	1.78	0.83
1:A:1018:ILE:HD11	1:A:1048:ALA:HB1	1.59	0.83
1:B:844:MSE:HE1	1:B:855:ASP:N	1.93	0.83
1:A:940:GLN:HA	1:A:940:GLN:OE1	1.77	0.82
1:B:1018:ILE:HD11	1:B:1048:ALA:HB1	1.59	0.82
1:B:1082:ARG:HB3	1:B:1082:ARG:HH11	1.42	0.82
1:A:844:MSE:CE	1:A:854:VAL:HB	2.09	0.82
1:B:617:TYR:O	1:B:621:ILE:HG12	1.78	0.82
1:A:844:MSE:HE1	1:A:855:ASP:N	1.95	0.81
1:A:785:GLU:CD	1:A:785:GLU:H	1.88	0.81
1:B:775:VAL:HG12	1:B:783:GLY:CA	2.11	0.81
1:A:929:TYR:O	1:A:932:TRP:HB2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1070:LYS:HG2	1:B:1075:THR:HB	1.63	0.80
1:B:1022:TRP:HE1	1:B:1050:TYR:HB2	1.46	0.80
1:B:605:VAL:HG21	1:B:857:TYR:CB	2.12	0.80
1:A:1082:ARG:HH11	1:A:1082:ARG:HB3	1.47	0.79
1:A:617:TYR:O	1:A:621:ILE:HG12	1.82	0.79
1:B:1082:ARG:HB3	1:B:1082:ARG:NH1	1.97	0.79
1:B:932:TRP:HZ3	1:B:957:TYR:CE2	2.01	0.79
1:A:874:GLU:CD	1:A:874:GLU:N	2.32	0.79
1:A:605:VAL:HG21	1:A:857:TYR:HB3	1.65	0.78
1:A:911:ASP:HB3	1:A:912:PRO:CD	2.13	0.78
1:B:962:LEU:HB3	1:B:991:LYS:NZ	1.98	0.78
1:B:864:ARG:HG2	1:B:864:ARG:HH11	1.48	0.78
1:A:1083:HIS:CE1	1:A:1085:LYS:HE2	2.19	0.78
1:B:1002:TRP:HZ2	1:B:1166:THR:HG21	1.48	0.78
1:B:1115:MSE:O	1:B:1119:VAL:HG23	1.83	0.78
1:B:1087:LYS:HE3	1:B:1087:LYS:HA	1.66	0.78
1:A:910:ARG:HB3	1:A:917:SER:HA	1.64	0.77
1:A:864:ARG:HG2	1:A:864:ARG:HH11	1.47	0.77
1:B:929:TYR:HB3	1:B:932:TRP:HB2	1.66	0.77
1:B:1108:GLU:O	1:B:1111:GLU:HG2	1.85	0.76
1:A:929:TYR:HB3	1:A:932:TRP:HB2	1.67	0.76
1:B:940:GLN:OE1	1:B:940:GLN:HA	1.83	0.76
1:A:932:TRP:HZ3	1:A:957:TYR:CE2	2.02	0.76
1:A:1082:ARG:HG2	1:A:1088:ASP:OD1	1.86	0.76
1:A:1097:TYR:HB2	1:A:1115:MSE:HE2	1.69	0.75
1:B:873:VAL:HG12	1:B:875:ALA:H	1.49	0.75
1:A:910:ARG:HB3	1:A:917:SER:CA	2.16	0.75
1:B:608:ILE:HD12	1:B:608:ILE:H	1.50	0.75
1:A:1087:LYS:HE3	1:A:1087:LYS:HA	1.69	0.75
1:B:784:ARG:HD2	1:B:820:PHE:HZ	1.48	0.75
1:B:761:HIS:HD2	1:B:770:GLN:HE21	1.33	0.74
1:B:929:TYR:O	1:B:932:TRP:HB2	1.85	0.74
1:A:960:VAL:HA	1:A:997:PHE:HE2	1.53	0.74
1:B:949:ASN:HD22	1:B:950:SER:N	1.86	0.74
1:B:1126:LYS:NZ	1:B:1126:LYS:HB3	2.02	0.74
1:A:1063:VAL:HA	1:A:1081:LEU:HD23	1.70	0.74
1:A:660:ASP:HB3	1:A:661:ILE:HD12	1.70	0.74
1:A:1044:GLN:H	1:A:1044:GLN:NE2	1.85	0.74
1:B:775:VAL:HG12	1:B:783:GLY:HA2	1.70	0.73
1:A:605:VAL:HG21	1:A:857:TYR:CB	2.18	0.73
1:B:930:ARG:HE	1:B:930:ARG:HA	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1002:TRP:HZ2	1:A:1166:THR:HG21	1.50	0.73
1:A:1022:TRP:NE1	1:A:1050:TYR:HB2	2.02	0.73
1:A:857:TYR:O	1:A:861:VAL:HG23	1.88	0.72
1:A:1142:ILE:HD13	1:A:1154:PHE:HD2	1.54	0.72
1:A:638:VAL:HG12	1:A:639:PHE:H	1.53	0.72
1:B:1038:GLU:OE1	1:B:1098:THR:HG23	1.88	0.72
1:A:1082:ARG:HB3	1:A:1082:ARG:NH1	2.03	0.72
1:A:911:ASP:O	1:A:913:PRO:CD	2.38	0.72
1:A:911:ASP:O	1:A:913:PRO:HD3	1.89	0.72
1:B:874:GLU:CD	1:B:874:GLU:N	2.44	0.72
1:B:1160:LEU:HD22	1:B:1170:VAL:HG13	1.68	0.72
1:B:841:ILE:HG22	1:B:845:LEU:HD11	1.71	0.72
1:A:775:VAL:HG12	1:A:783:GLY:HA2	1.71	0.71
1:B:721:THR:HG22	1:B:785:GLU:O	1.90	0.71
1:B:1022:TRP:NE1	1:B:1050:TYR:HB2	2.05	0.71
1:A:721:THR:HG22	1:A:785:GLU:O	1.90	0.71
1:A:1070:LYS:HG2	1:A:1075:THR:HB	1.71	0.71
1:A:775:VAL:HG12	1:A:783:GLY:CA	2.20	0.71
1:A:909:LYS:HD2	1:A:909:LYS:C	2.15	0.71
1:A:949:ASN:HD22	1:A:949:ASN:C	1.99	0.71
1:A:617:TYR:CE2	1:A:621:ILE:HD13	2.25	0.71
1:A:841:ILE:HG22	1:A:845:LEU:HD11	1.73	0.71
1:B:660:ASP:HB3	1:B:661:ILE:HD12	1.72	0.70
1:B:1063:VAL:HA	1:B:1081:LEU:HD23	1.74	0.70
1:A:963:LYS:HE3	1:A:1027:GLN:HB3	1.74	0.70
1:A:1153:ILE:CD1	1:A:1192:GLN:HB3	2.19	0.70
1:A:1038:GLU:OE1	1:A:1098:THR:HG23	1.91	0.70
1:A:949:ASN:HD22	1:A:950:SER:N	1.90	0.69
1:B:1120:LYS:HA	1:B:1123:LEU:HD12	1.74	0.69
1:A:864:ARG:HG2	1:A:864:ARG:NH1	2.07	0.69
1:B:1061:ILE:HD12	1:B:1061:ILE:C	2.17	0.69
1:A:1061:ILE:C	1:A:1061:ILE:HD12	2.18	0.69
1:A:1160:LEU:HD22	1:A:1170:VAL:HG13	1.74	0.69
1:B:1014:LEU:C	1:B:1016:GLU:H	2.01	0.69
1:A:930:ARG:HA	1:A:930:ARG:HE	1.58	0.69
1:B:947:ASN:ND2	1:B:992:TYR:OH	2.24	0.69
1:A:1073:THR:HG22	1:A:1111:GLU:CD	2.18	0.69
1:A:937:ILE:HG12	1:A:956:ASP:OD1	1.92	0.69
1:B:952:VAL:HG11	1:B:1146:ASP:HB2	1.75	0.68
1:B:874:GLU:O	1:B:878:ILE:HG13	1.92	0.68
1:A:1172:ILE:O	1:A:1176:VAL:HG23	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:954:PRO:HD3	1:B:994:ASN:OD1	1.92	0.68
1:A:1014:LEU:C	1:A:1016:GLU:H	2.02	0.68
1:A:1077:ARG:HE	1:A:1094:GLN:HE22	1.42	0.68
1:B:617:TYR:CE2	1:B:621:ILE:HD13	2.29	0.68
1:A:734:ARG:NH1	1:A:735:ASN:H	1.92	0.68
1:B:911:ASP:HB2	1:B:912:PRO:CD	2.24	0.67
1:A:599:GLU:HA	1:A:865:ARG:HH21	1.59	0.67
1:B:864:ARG:HG2	1:B:864:ARG:NH1	2.07	0.67
1:A:661:ILE:HD12	1:A:661:ILE:N	2.10	0.67
1:B:1063:VAL:HG12	1:B:1081:LEU:HD21	1.77	0.67
1:B:796:ASP:OD1	1:B:797:HIS:ND1	2.18	0.67
1:B:929:TYR:CE2	1:B:1181:LYS:HE3	2.30	0.67
1:B:1153:ILE:CD1	1:B:1192:GLN:HB3	2.22	0.67
1:B:809:LEU:O	1:B:813:VAL:HG22	1.94	0.66
1:A:806:LEU:HD23	1:A:841:ILE:HD11	1.77	0.66
1:A:608:ILE:HD12	1:A:608:ILE:H	1.59	0.66
1:B:844:MSE:HE1	1:B:854:VAL:C	2.20	0.66
1:B:1044:GLN:H	1:B:1044:GLN:HE21	1.42	0.66
1:B:932:TRP:CE3	1:B:933:ARG:HG3	2.30	0.66
1:B:948:ARG:HH12	1:B:1045:GLU:HG3	1.61	0.65
1:B:1142:ILE:HD13	1:B:1154:PHE:HD2	1.61	0.65
1:B:769:ILE:HG12	1:B:789:ILE:HG23	1.78	0.65
1:B:940:GLN:O	1:B:944:LYS:HG2	1.96	0.65
1:A:895:VAL:HG21	1:A:900:LEU:HA	1.76	0.65
1:A:909:LYS:HD2	1:A:909:LYS:O	1.97	0.65
1:A:952:VAL:HG11	1:A:1146:ASP:HB2	1.78	0.65
1:B:616:THR:O	1:B:620:LYS:HG2	1.96	0.65
1:A:940:GLN:O	1:A:944:LYS:HG2	1.95	0.65
1:A:1063:VAL:HA	1:A:1081:LEU:CD2	2.27	0.65
1:A:796:ASP:OD1	1:A:797:HIS:ND1	2.20	0.65
1:A:696:LYS:HD3	1:A:697:TYR:CZ	2.32	0.64
1:B:937:ILE:HG12	1:B:956:ASP:OD1	1.97	0.64
1:B:1183:ARG:HB3	1:B:1186:MSE:HE2	1.78	0.64
1:A:841:ILE:HG22	1:A:845:LEU:CD1	2.28	0.64
1:B:696:LYS:HD3	1:B:697:TYR:CZ	2.33	0.64
1:B:959:ARG:O	1:B:961:PRO:HD3	1.96	0.64
1:B:638:VAL:HG12	1:B:639:PHE:H	1.63	0.64
1:B:1098:THR:O	1:B:1100:TRP:N	2.30	0.64
1:A:704:ARG:H	1:A:707:THR:HB	1.61	0.64
1:A:731:GLU:OE2	1:A:796:ASP:HB2	1.98	0.64
1:B:1189:THR:HB	1:B:1191:GLU:OE1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:VAL:HG12	1:A:1081:LEU:HD21	1.79	0.64
1:B:704:ARG:H	1:B:707:THR:HB	1.63	0.64
1:A:1041:HIS:HB3	1:A:1044:GLN:HG2	1.78	0.64
1:B:731:GLU:OE2	1:B:796:ASP:HB2	1.98	0.64
1:A:878:ILE:O	1:A:882:GLN:HG3	1.97	0.64
1:B:962:LEU:HB3	1:B:991:LYS:HG2	1.79	0.64
1:B:794:TRP:NE1	1:B:834:ARG:HG2	2.13	0.63
1:A:951:ASN:O	1:A:1184:LEU:HD12	1.99	0.63
1:B:906:ASN:O	1:B:909:LYS:HG3	1.98	0.63
1:A:728:ARG:HG2	1:A:792:THR:HG22	1.80	0.63
1:B:958:ASN:O	1:B:997:PHE:HD2	1.81	0.63
1:B:1114:SER:HA	1:B:1117:GLN:HG2	1.80	0.63
1:A:1081:LEU:O	1:A:1089:SER:HA	1.99	0.63
1:B:1039:LEU:HD13	1:B:1049:GLN:HE21	1.64	0.63
1:A:1102:VAL:HB	1:A:1149:GLN:HE21	1.63	0.63
1:B:844:MSE:HE2	1:B:856:VAL:N	2.14	0.63
1:A:789:ILE:CG1	1:A:816:PHE:HE2	2.12	0.62
1:A:1186:MSE:O	1:A:1187:VAL:C	2.42	0.62
1:B:1039:LEU:HD22	1:B:1048:ALA:O	1.99	0.62
1:A:962:LEU:O	1:A:991:LYS:HB2	1.99	0.62
1:B:631:GLU:O	1:B:857:TYR:HE1	1.82	0.62
1:B:992:TYR:C	1:B:992:TYR:CD2	2.77	0.62
1:B:1101:SER:C	1:B:1103:GLU:H	2.06	0.62
1:B:605:VAL:CG2	1:B:857:TYR:HB3	2.27	0.62
1:B:808:LYS:HE2	1:B:894:GLU:OE2	1.99	0.62
1:B:841:ILE:HG22	1:B:845:LEU:CD1	2.29	0.62
1:B:1128:SER:O	1:B:1129:SER:HB2	1.99	0.62
1:B:1002:TRP:CZ2	1:B:1166:THR:HG21	2.33	0.62
1:A:1101:SER:C	1:A:1103:GLU:H	2.06	0.62
1:B:774:ILE:O	1:B:783:GLY:HA2	2.00	0.62
1:B:942:GLU:N	1:B:942:GLU:OE1	2.33	0.62
1:A:958:ASN:O	1:A:997:PHE:HD2	1.83	0.61
1:B:912:PRO:HB2	1:B:915:GLU:CG	2.22	0.61
1:B:734:ARG:NH1	1:B:735:ASN:H	1.98	0.61
1:A:1179:LEU:HB3	1:A:1186:MSE:HG3	1.82	0.61
1:B:777:LYS:HZ2	1:B:781:ALA:HB3	1.63	0.61
1:B:1021:PHE:O	1:B:1025:ILE:HG23	2.00	0.61
1:A:631:GLU:O	1:A:857:TYR:HE1	1.83	0.61
1:A:844:MSE:HE2	1:A:856:VAL:N	2.16	0.61
1:A:873:VAL:HG12	1:A:875:ALA:N	2.13	0.61
1:A:1108:GLU:O	1:A:1111:GLU:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1148:SER:HB3	1:B:1185:GLY:C	2.26	0.61
1:B:1157:LEU:HD21	1:B:1199:VAL:HG21	1.83	0.61
1:B:938:GLY:HA2	1:B:992:TYR:CE1	2.36	0.61
1:A:922:GLU:N	1:A:925:ARG:HH21	1.99	0.61
1:A:1002:TRP:CZ2	1:A:1166:THR:HG21	2.35	0.61
1:B:626:ARG:N	1:B:627:PRO:CD	2.64	0.61
1:B:864:ARG:HD2	1:B:870:MSE:H	1.66	0.61
1:B:805:LEU:O	1:B:808:LYS:HB3	2.01	0.60
1:B:1199:VAL:O	1:B:1203:THR:HG23	2.01	0.60
1:A:605:VAL:CG2	1:A:857:TYR:HB3	2.31	0.60
1:A:1098:THR:O	1:A:1100:TRP:N	2.33	0.60
1:B:949:ASN:HD22	1:B:949:ASN:C	2.07	0.60
1:B:1121:GLN:O	1:B:1121:GLN:HG2	1.99	0.60
1:A:1039:LEU:HD13	1:A:1049:GLN:HG3	1.83	0.60
1:A:615:GLU:O	1:A:616:THR:C	2.44	0.60
1:A:1014:LEU:C	1:A:1016:GLU:N	2.58	0.60
1:B:806:LEU:HD23	1:B:841:ILE:HD11	1.82	0.60
1:A:794:TRP:NE1	1:A:834:ARG:HG2	2.17	0.60
1:B:602:LEU:N	1:B:602:LEU:HD22	2.15	0.60
1:B:1161:LEU:O	1:B:1165:GLU:HG2	2.02	0.60
1:A:1077:ARG:NE	1:A:1094:GLN:HE22	1.99	0.60
1:B:942:GLU:HG2	1:B:943:ASN:ND2	2.16	0.60
1:B:1024:MSE:HE3	1:B:1141:LEU:HD11	1.83	0.60
1:B:881:HIS:O	1:B:885:VAL:HG23	2.01	0.60
1:B:991:LYS:H	1:B:991:LYS:HD3	1.65	0.60
1:B:1073:THR:HG22	1:B:1111:GLU:CD	2.27	0.60
1:A:626:ARG:N	1:A:627:PRO:CD	2.65	0.60
1:A:870:MSE:O	1:A:871:VAL:C	2.45	0.60
1:B:960:VAL:HA	1:B:997:PHE:HE2	1.67	0.59
1:A:760:GLN:HB2	1:A:771:LYS:HB2	1.84	0.59
1:A:874:GLU:O	1:A:878:ILE:HG13	2.02	0.59
1:B:857:TYR:O	1:B:861:VAL:HG23	2.02	0.59
1:B:1040:LYS:CB	1:B:1045:GLU:HA	2.27	0.59
1:B:1183:ARG:O	1:B:1186:MSE:HG2	2.01	0.59
1:B:765:PRO:HG2	1:B:1001:TYR:CZ	2.37	0.59
1:B:844:MSE:HE2	1:B:856:VAL:CA	2.31	0.59
1:A:805:LEU:O	1:A:808:LYS:HB3	2.03	0.59
1:B:689:ASP:H	1:B:866:GLN:HE22	1.49	0.59
1:B:777:LYS:HD3	1:B:781:ALA:HB2	1.82	0.59
1:B:1160:LEU:HD23	1:B:1175:VAL:HG21	1.85	0.59
1:A:960:VAL:HA	1:A:997:PHE:CE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1014:LEU:C	1:B:1016:GLU:N	2.57	0.59
1:B:1097:TYR:HB2	1:B:1115:MSE:HE2	1.85	0.59
1:A:932:TRP:CE3	1:A:933:ARG:HG3	2.37	0.59
1:B:1077:ARG:HE	1:B:1094:GLN:HE22	1.50	0.59
1:B:901:HIS:HB2	1:B:902:PRO:HD3	1.85	0.59
1:B:870:MSE:O	1:B:871:VAL:C	2.44	0.58
1:A:810:ARG:HD3	1:A:814:ASN:OD1	2.02	0.58
1:A:1039:LEU:HD13	1:A:1049:GLN:HE21	1.68	0.58
1:B:929:TYR:O	1:B:930:ARG:C	2.47	0.58
1:B:946:LYS:C	1:B:947:ASN:HD22	2.11	0.58
1:A:769:ILE:HG12	1:A:789:ILE:HG23	1.85	0.58
1:B:778:LYS:HE2	1:B:778:LYS:HA	1.85	0.58
1:B:926:LEU:HD11	1:B:1193:TYR:CE1	2.38	0.58
1:A:601:GLN:HA	1:A:601:GLN:OE1	2.04	0.58
1:B:1015:LYS:HA	1:B:1018:ILE:HG13	1.84	0.58
1:A:700:ALA:O	1:A:827:HIS:HB2	2.03	0.58
1:B:873:VAL:HG12	1:B:875:ALA:N	2.17	0.58
1:A:1039:LEU:HD22	1:A:1048:ALA:O	2.03	0.58
1:B:700:ALA:O	1:B:827:HIS:HB2	2.03	0.58
1:B:1013:PRO:HD2	1:B:1047:CYS:SG	2.44	0.58
1:B:904:LEU:HG	1:B:908:LYS:HE2	1.85	0.58
1:B:1063:VAL:HA	1:B:1081:LEU:CD2	2.33	0.58
1:B:1082:ARG:HG2	1:B:1088:ASP:OD1	2.03	0.58
1:B:1105:LEU:O	1:B:1106:PRO:C	2.47	0.58
1:A:638:VAL:HG12	1:A:639:PHE:N	2.19	0.58
1:B:1172:ILE:O	1:B:1176:VAL:HG23	2.04	0.57
1:B:615:GLU:O	1:B:616:THR:C	2.47	0.57
1:B:615:GLU:HA	1:B:618:LYS:HB2	1.86	0.57
1:B:844:MSE:HE2	1:B:856:VAL:CG2	2.33	0.57
1:A:616:THR:O	1:A:620:LYS:HG2	2.05	0.57
1:A:794:TRP:CZ3	1:A:806:LEU:HD11	2.39	0.57
1:B:791:PHE:CD2	1:B:794:TRP:HB2	2.39	0.57
1:B:906:ASN:C	1:B:908:LYS:H	2.12	0.57
1:B:878:ILE:O	1:B:882:GLN:HG3	2.05	0.57
1:A:1144:CYS:O	1:A:1145:ARG:C	2.46	0.57
1:A:1189:THR:HB	1:A:1191:GLU:OE1	2.05	0.57
1:B:929:TYR:HD2	1:B:932:TRP:CD1	2.21	0.57
1:B:1186:MSE:O	1:B:1187:VAL:C	2.46	0.57
1:B:962:LEU:O	1:B:991:LYS:HD3	2.04	0.57
1:A:844:MSE:HE2	1:A:856:VAL:CA	2.34	0.57
1:B:906:ASN:C	1:B:908:LYS:N	2.62	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:926:LEU:HG	1:B:1173:PHE:CE1	2.39	0.57
1:A:602:LEU:HB2	1:A:857:TYR:OH	2.05	0.57
1:A:615:GLU:OE2	1:A:615:GLU:N	2.33	0.57
1:A:844:MSE:HE2	1:A:856:VAL:CG2	2.35	0.57
1:A:942:GLU:HG2	1:A:943:ASN:ND2	2.19	0.57
1:A:1015:LYS:NZ	1:A:1015:LYS:HB3	2.19	0.57
1:A:1157:LEU:HD21	1:A:1199:VAL:HG21	1.87	0.57
1:A:649:LYS:HD3	1:A:651:PHE:CZ	2.39	0.57
1:A:911:ASP:O	1:A:913:PRO:N	2.38	0.57
1:A:698:ILE:HG13	1:A:823:PRO:HB2	1.87	0.56
1:A:844:MSE:HE1	1:A:854:VAL:C	2.29	0.56
1:A:890:PHE:CE2	1:A:927:PRO:HD3	2.40	0.56
1:A:1088:ASP:O	1:A:1089:SER:C	2.47	0.56
1:B:1088:ASP:O	1:B:1089:SER:C	2.48	0.56
1:A:761:HIS:CD2	1:A:770:GLN:HE21	2.09	0.56
1:A:765:PRO:HG2	1:A:1001:TYR:CZ	2.40	0.56
1:A:804:HIS:CD2	1:A:1174:GLN:HG3	2.40	0.56
1:B:922:GLU:N	1:B:925:ARG:HH21	2.03	0.56
1:B:1011:GLN:HB2	1:B:1145:ARG:O	2.05	0.56
1:B:1013:PRO:HG3	1:B:1050:TYR:CD2	2.40	0.56
1:B:1102:VAL:HB	1:B:1149:GLN:HE21	1.70	0.56
1:A:869:LEU:O	1:A:870:MSE:O	2.24	0.56
1:B:948:ARG:NH2	1:B:1047:CYS:HA	2.21	0.56
1:A:673:GLU:HG2	1:A:681:ASN:HB3	1.87	0.56
1:A:881:HIS:O	1:A:885:VAL:HG23	2.06	0.56
1:B:1179:LEU:HD22	1:B:1186:MSE:HE3	1.86	0.56
1:A:947:ASN:HD21	1:A:992:TYR:HE2	1.52	0.56
1:A:844:MSE:HE2	1:A:856:VAL:HG23	1.87	0.56
1:A:942:GLU:N	1:A:942:GLU:OE1	2.39	0.56
1:A:1015:LYS:HA	1:A:1018:ILE:HG13	1.88	0.56
1:A:734:ARG:NH1	1:A:735:ASN:N	2.53	0.56
1:B:831:GLY:HA2	1:B:835:THR:HG21	1.88	0.56
1:A:1044:GLN:H	1:A:1044:GLN:HE21	1.52	0.56
1:A:1097:TYR:CE2	1:A:1112:LEU:HD23	2.41	0.56
1:A:938:GLY:HA3	1:A:953:ILE:CG2	2.36	0.55
1:A:1142:ILE:HD13	1:A:1154:PHE:CD2	2.40	0.55
1:A:1017:THR:C	1:A:1019:GLY:N	2.64	0.55
1:B:728:ARG:HG2	1:B:792:THR:HG22	1.87	0.55
1:B:777:LYS:HZ3	1:B:781:ALA:HB3	1.66	0.55
1:B:897:LEU:HG	1:B:1168:GLU:HA	1.89	0.55
1:B:955:TYR:OH	1:B:1184:LEU:HD23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1049:GLN:O	1:B:1051:TRP:N	2.39	0.55
1:A:929:TYR:HD2	1:A:932:TRP:CD1	2.24	0.55
1:B:726:VAL:O	1:B:726:VAL:HG12	2.05	0.55
1:A:789:ILE:HD12	1:A:789:ILE:H	1.72	0.55
1:A:789:ILE:HG12	1:A:816:PHE:HE2	1.71	0.55
1:A:907:MSE:O	1:A:918:PRO:HD2	2.06	0.55
1:B:621:ILE:HG23	1:B:628:PHE:HE2	1.71	0.55
1:A:949:ASN:C	1:A:949:ASN:ND2	2.65	0.55
1:B:964:HIS:O	1:B:965:GLU:C	2.48	0.55
1:A:614:LEU:HD23	1:A:889:GLN:NE2	2.22	0.55
1:B:1160:LEU:CD2	1:B:1175:VAL:HG21	2.37	0.55
1:A:804:HIS:NE2	1:A:1174:GLN:HG3	2.22	0.55
1:A:1148:SER:HB3	1:A:1185:GLY:HA3	1.88	0.55
1:B:687:TYR:CG	1:B:695:ARG:HD2	2.41	0.55
1:B:801:GLU:CD	1:B:801:GLU:H	2.15	0.55
1:A:1014:LEU:O	1:A:1016:GLU:N	2.40	0.55
1:A:734:ARG:HH12	1:A:735:ASN:H	1.53	0.55
1:B:768:ILE:HG12	1:B:790:GLN:HB3	1.89	0.55
1:B:991:LYS:H	1:B:991:LYS:CD	2.20	0.55
1:B:1132:ASN:N	1:B:1132:ASN:HD22	2.04	0.55
1:A:962:LEU:HB3	1:A:991:LYS:CB	2.37	0.54
1:B:960:VAL:HA	1:B:997:PHE:CE2	2.42	0.54
1:A:962:LEU:HD11	1:A:1020:ASP:HB3	1.90	0.54
1:A:963:LYS:HZ2	1:A:963:LYS:HB2	1.73	0.54
1:B:895:VAL:HG22	1:B:896:ASN:N	2.14	0.54
1:A:689:ASP:H	1:A:866:GLN:HE22	1.55	0.54
1:B:869:LEU:O	1:B:870:MSE:O	2.26	0.54
1:A:870:MSE:O	1:A:872:GLN:N	2.40	0.54
1:A:1046:ILE:HG23	1:A:1145:ARG:HG2	1.89	0.54
1:B:756:VAL:HG22	1:B:774:ILE:HG22	1.88	0.54
1:B:1157:LEU:HD21	1:B:1199:VAL:CG2	2.37	0.54
1:A:1105:LEU:O	1:A:1106:PRO:C	2.51	0.54
1:B:713:ARG:O	1:B:717:GLU:HG3	2.06	0.54
1:A:929:TYR:HB3	1:A:932:TRP:CB	2.37	0.54
1:B:657:ARG:NH1	1:B:704:ARG:HG2	2.23	0.54
1:B:760:GLN:HB2	1:B:771:LYS:HB2	1.90	0.54
1:B:894:GLU:HG2	1:B:1169:VAL:HG22	1.89	0.54
1:A:948:ARG:HH12	1:A:1045:GLU:HG3	1.72	0.54
1:A:1114:SER:HA	1:A:1117:GLN:HG2	1.90	0.54
1:B:929:TYR:HE2	1:B:1181:LYS:HE3	1.71	0.54
1:B:1144:CYS:O	1:B:1145:ARG:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:SER:OG	1:B:746:GLU:HG2	2.08	0.54
1:B:813:VAL:C	1:B:815:ALA:H	2.16	0.54
1:B:844:MSE:HE2	1:B:856:VAL:HG23	1.89	0.54
1:B:962:LEU:CB	1:B:991:LYS:HG2	2.36	0.54
1:B:1113:ILE:HG13	1:B:1203:THR:HG21	1.88	0.54
1:A:615:GLU:HA	1:A:618:LYS:HB2	1.89	0.54
1:A:901:HIS:HB2	1:A:902:PRO:HD3	1.89	0.54
1:B:649:LYS:HD3	1:B:651:PHE:CZ	2.42	0.54
1:B:789:ILE:HD12	1:B:789:ILE:H	1.73	0.54
1:B:810:ARG:HD3	1:B:814:ASN:OD1	2.08	0.54
1:B:909:LYS:HD2	1:B:909:LYS:O	2.08	0.54
1:B:929:TYR:HB3	1:B:932:TRP:CB	2.36	0.54
1:A:1157:LEU:HD21	1:A:1199:VAL:CG2	2.38	0.54
1:B:1081:LEU:O	1:B:1089:SER:HA	2.08	0.54
1:A:791:PHE:CD2	1:A:794:TRP:HB2	2.42	0.53
1:A:918:PRO:O	1:A:921:ALA:HB3	2.08	0.53
1:B:1063:VAL:HG12	1:B:1081:LEU:CD2	2.39	0.53
1:A:599:GLU:HA	1:A:865:ARG:NH2	2.23	0.53
1:A:801:GLU:CD	1:A:801:GLU:H	2.15	0.53
1:A:831:GLY:HA2	1:A:835:THR:HG21	1.89	0.53
1:A:1121:GLN:O	1:A:1121:GLN:HG2	2.04	0.53
1:B:1025:ILE:HD11	1:B:1081:LEU:CD1	2.38	0.53
1:A:768:ILE:HG12	1:A:790:GLN:HB3	1.90	0.53
1:A:929:TYR:CE2	1:A:1181:LYS:HE3	2.43	0.53
1:A:1179:LEU:CD2	1:A:1186:MSE:HE3	2.18	0.53
1:A:726:VAL:HG12	1:A:726:VAL:O	2.07	0.53
1:A:774:ILE:O	1:A:783:GLY:HA2	2.08	0.53
1:A:1021:PHE:O	1:A:1025:ILE:HG23	2.08	0.53
1:A:1046:ILE:HG23	1:A:1145:ARG:HE	1.74	0.53
1:B:929:TYR:HB3	1:B:932:TRP:CG	2.44	0.53
1:B:954:PRO:HD3	1:B:994:ASN:CG	2.34	0.53
1:B:1018:ILE:HG23	1:B:1050:TYR:HA	1.89	0.53
1:B:1070:LYS:HG2	1:B:1075:THR:CB	2.35	0.53
1:B:775:VAL:HG12	1:B:783:GLY:HA3	1.88	0.53
1:B:1049:GLN:C	1:B:1051:TRP:H	2.16	0.53
1:A:869:LEU:O	1:A:869:LEU:HG	2.09	0.53
1:B:1041:HIS:HB3	1:B:1044:GLN:HG2	1.91	0.53
1:A:958:ASN:O	1:A:959:ARG:C	2.51	0.53
1:A:1018:ILE:HG23	1:A:1050:TYR:HA	1.91	0.53
1:B:794:TRP:CZ3	1:B:806:LEU:HD11	2.44	0.53
1:B:894:GLU:O	1:B:895:VAL:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:LEU:HD22	1:B:885:VAL:CG1	2.39	0.53
1:B:844:MSE:CE	1:B:856:VAL:N	2.72	0.53
1:B:855:ASP:OD2	1:B:858:GLY:HA3	2.09	0.53
1:B:911:ASP:CB	1:B:912:PRO:HD3	2.30	0.53
1:B:1014:LEU:O	1:B:1016:GLU:N	2.42	0.53
1:B:1061:ILE:HD12	1:B:1061:ILE:O	2.08	0.53
1:A:1203:THR:O	1:A:1204:TYR:CD1	2.62	0.52
1:B:621:ILE:O	1:B:625:GLY:N	2.42	0.52
1:B:707:THR:HG22	1:B:707:THR:O	2.10	0.52
1:A:611:ASP:OD1	1:A:612:ILE:HG23	2.10	0.52
1:A:960:VAL:HG22	1:A:997:PHE:CE2	2.45	0.52
1:B:661:ILE:HD12	1:B:661:ILE:N	2.23	0.52
1:B:820:PHE:CD1	1:B:820:PHE:N	2.77	0.52
1:B:908:LYS:O	1:B:917:SER:HB2	2.09	0.52
1:B:1025:ILE:HD12	1:B:1025:ILE:O	2.09	0.52
1:B:1028:ARG:HG3	1:B:1028:ARG:HH11	1.74	0.52
1:A:946:LYS:C	1:A:947:ASN:HD22	2.17	0.52
1:B:1126:LYS:HB3	1:B:1126:LYS:HZ2	1.70	0.52
1:A:621:ILE:HG23	1:A:628:PHE:HE2	1.75	0.52
1:A:692:LYS:O	1:A:693:GLU:C	2.52	0.52
1:A:1049:GLN:O	1:A:1051:TRP:N	2.43	0.52
1:B:608:ILE:HD12	1:B:608:ILE:N	2.19	0.52
1:B:692:LYS:O	1:B:693:GLU:C	2.53	0.52
1:B:1136:LYS:HD2	1:B:1136:LYS:N	2.25	0.52
1:A:1040:LYS:CB	1:A:1045:GLU:HA	2.33	0.52
1:A:715:ILE:CD1	1:A:825:VAL:HG21	2.40	0.52
1:B:741:TRP:HB2	1:B:742:PRO:HD2	1.92	0.52
1:B:922:GLU:CA	1:B:925:ARG:HH21	2.23	0.52
1:A:812:ARG:O	1:A:815:ALA:HB3	2.09	0.52
1:B:791:PHE:CE2	1:B:794:TRP:HB2	2.44	0.52
1:B:806:LEU:HA	1:B:809:LEU:CD2	2.40	0.52
1:A:1160:LEU:HD23	1:A:1175:VAL:HG21	1.92	0.51
1:B:930:ARG:HG3	1:B:931:SER:N	2.25	0.51
1:A:608:ILE:O	1:A:853:LYS:HA	2.11	0.51
1:A:1013:PRO:HG3	1:A:1050:TYR:CD2	2.44	0.51
1:B:618:LYS:O	1:B:621:ILE:HG13	2.10	0.51
1:B:897:LEU:HG	1:B:1168:GLU:CA	2.40	0.51
1:A:743:SER:OG	1:A:746:GLU:HG2	2.10	0.51
1:A:880:ILE:O	1:A:883:ALA:HB3	2.09	0.51
1:A:1055:LYS:HE3	1:A:1062:GLU:OE1	2.11	0.51
1:B:895:VAL:HG21	1:B:900:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:929:TYR:OH	1:B:1177:LYS:HE2	2.10	0.51
1:A:930:ARG:HG3	1:A:931:SER:N	2.24	0.51
1:B:1017:THR:O	1:B:1019:GLY:N	2.44	0.51
1:B:1083:HIS:NE2	1:B:1085:LYS:HE2	2.25	0.51
1:A:994:ASN:OD1	1:A:1183:ARG:NH2	2.44	0.51
1:B:649:LYS:HD3	1:B:651:PHE:HZ	1.76	0.51
1:B:907:MSE:O	1:B:918:PRO:HD2	2.11	0.51
1:B:953:ILE:HA	1:B:994:ASN:HD21	1.75	0.51
1:A:614:LEU:HD22	1:A:885:VAL:CG1	2.41	0.51
1:A:929:TYR:HB3	1:A:932:TRP:CG	2.46	0.51
1:A:1011:GLN:HB2	1:A:1145:ARG:O	2.10	0.51
1:B:901:HIS:CB	1:B:902:PRO:HD3	2.40	0.51
1:B:1044:GLN:HE21	1:B:1044:GLN:N	2.08	0.51
1:B:1077:ARG:NE	1:B:1094:GLN:HE22	2.08	0.51
1:B:1141:LEU:HD23	1:B:1141:LEU:C	2.36	0.51
1:A:764:CYS:HB3	1:A:765:PRO:CD	2.40	0.51
1:A:929:TYR:O	1:A:930:ARG:C	2.54	0.51
1:B:863:LEU:C	1:B:865:ARG:H	2.19	0.51
1:B:1192:GLN:O	1:B:1195:PHE:HB3	2.11	0.51
1:B:734:ARG:HH12	1:B:735:ASN:H	1.57	0.51
1:B:1142:ILE:HD13	1:B:1154:PHE:CD2	2.45	0.51
1:A:657:ARG:NH2	1:A:737:CYS:HA	2.25	0.50
1:A:818:ASN:O	1:A:820:PHE:N	2.44	0.50
1:A:748:THR:OG1	1:A:757:LYS:HG3	2.11	0.50
1:A:910:ARG:HD3	1:A:915:GLU:O	2.11	0.50
1:A:1153:ILE:HD13	1:A:1187:VAL:HG22	1.93	0.50
1:A:1026:PHE:CE2	1:A:1090:ARG:NH1	2.79	0.50
1:A:1101:SER:C	1:A:1103:GLU:N	2.70	0.50
1:B:684:ASN:OD1	1:B:867:ARG:NH2	2.38	0.50
1:B:1101:SER:HB3	1:B:1103:GLU:OE1	2.11	0.50
1:A:958:ASN:C	1:A:959:ARG:O	2.54	0.50
1:B:1017:THR:C	1:B:1019:GLY:N	2.65	0.50
1:B:1141:LEU:HD23	1:B:1142:ILE:N	2.27	0.50
1:A:801:GLU:OE1	1:A:805:LEU:CD1	2.60	0.50
1:B:1087:LYS:HE3	1:B:1087:LYS:CA	2.40	0.50
1:A:599:GLU:CA	1:A:865:ARG:HH21	2.24	0.50
1:A:641:LYS:O	1:A:643:PRO:HD3	2.11	0.50
1:A:791:PHE:CE2	1:A:794:TRP:HB2	2.47	0.50
1:A:863:LEU:C	1:A:865:ARG:H	2.18	0.50
1:A:1113:ILE:HG13	1:A:1203:THR:HG21	1.93	0.50
1:B:608:ILE:H	1:B:608:ILE:CD1	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1039:LEU:HD13	1:B:1049:GLN:HG3	1.93	0.50
1:A:947:ASN:ND2	1:A:994:ASN:HD22	2.09	0.50
1:A:1004:PRO:O	1:A:1006:VAL:HG23	2.11	0.50
1:A:1029:LYS:HA	1:A:1090:ARG:NH2	2.27	0.50
1:A:713:ARG:O	1:A:717:GLU:HG3	2.11	0.50
1:A:716:TRP:O	1:A:784:ARG:NH2	2.44	0.50
1:B:698:ILE:HG13	1:B:823:PRO:HB2	1.94	0.50
1:B:768:ILE:O	1:B:768:ILE:HG13	2.12	0.50
1:B:873:VAL:CG1	1:B:875:ALA:H	2.23	0.50
1:A:904:LEU:HG	1:A:908:LYS:HE2	1.94	0.50
1:A:1014:LEU:O	1:A:1017:THR:N	2.43	0.50
1:B:638:VAL:HG12	1:B:639:PHE:N	2.25	0.50
1:B:831:GLY:C	1:B:835:THR:HG21	2.37	0.50
1:B:901:HIS:NE2	1:B:1205:PRO:HA	2.27	0.50
1:B:1000:SER:HB3	1:B:1005:GLU:O	2.12	0.50
1:B:1131:GLY:O	1:B:1132:ASN:HB3	2.12	0.50
1:A:926:LEU:HG	1:A:1173:PHE:CE1	2.47	0.49
1:B:803:PRO:O	1:B:807:LEU:HD13	2.12	0.49
1:A:684:ASN:OD1	1:A:867:ARG:NH2	2.40	0.49
1:B:712:TRP:CE2	1:B:756:VAL:HG21	2.47	0.49
1:B:1043:ASP:HB2	1:B:1044:GLN:NE2	2.28	0.49
1:B:1101:SER:C	1:B:1103:GLU:N	2.71	0.49
1:B:716:TRP:O	1:B:784:ARG:NH2	2.44	0.49
1:B:1020:ASP:HA	1:B:1023:GLN:OE1	2.13	0.49
1:A:657:ARG:NH1	1:A:704:ARG:HG2	2.27	0.49
1:A:922:GLU:CA	1:A:925:ARG:HH21	2.25	0.49
1:A:1017:THR:O	1:A:1019:GLY:N	2.45	0.49
1:B:613:LEU:HD23	1:B:888:ASN:OD1	2.12	0.49
1:B:644:ILE:HG12	1:B:664:TYR:HA	1.94	0.49
1:B:687:TYR:CD2	1:B:695:ARG:HD2	2.48	0.49
1:B:697:TYR:CE1	1:B:839:ILE:HG23	2.47	0.49
1:B:929:TYR:CE2	1:B:1181:LYS:HG3	2.47	0.49
1:B:1179:LEU:O	1:B:1180:ARG:C	2.55	0.49
1:A:897:LEU:HG	1:A:1168:GLU:O	2.13	0.49
1:A:962:LEU:HB3	1:A:991:LYS:HB3	1.95	0.49
1:B:1002:TRP:O	1:B:1005:GLU:HG2	2.13	0.49
1:A:599:GLU:HB3	1:A:865:ARG:NH2	2.28	0.49
1:A:844:MSE:CE	1:A:856:VAL:N	2.75	0.49
1:A:1049:GLN:C	1:A:1051:TRP:H	2.20	0.49
1:A:1141:LEU:HD23	1:A:1142:ILE:N	2.27	0.49
1:A:1160:LEU:CD2	1:A:1175:VAL:HG21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1014:LEU:O	1:B:1017:THR:N	2.42	0.49
1:B:1083:HIS:CE1	1:B:1085:LYS:HB3	2.47	0.49
1:A:649:LYS:HD3	1:A:651:PHE:HZ	1.75	0.49
1:A:764:CYS:HB3	1:A:765:PRO:HD2	1.95	0.49
1:A:801:GLU:OE1	1:A:805:LEU:HD11	2.13	0.49
1:A:813:VAL:C	1:A:815:ALA:H	2.19	0.49
1:B:870:MSE:O	1:B:872:GLN:N	2.45	0.49
1:B:1187:VAL:HG13	1:B:1192:GLN:HB2	1.95	0.49
1:A:926:LEU:HD11	1:A:1193:TYR:CE1	2.48	0.49
1:B:848:LEU:HD23	1:B:852:ASN:HA	1.93	0.49
1:B:1015:LYS:NZ	1:B:1015:LYS:HB3	2.28	0.49
1:B:1097:TYR:OH	1:B:1111:GLU:HG3	2.13	0.49
1:A:806:LEU:HD23	1:A:841:ILE:CD1	2.42	0.49
1:A:806:LEU:C	1:A:808:LYS:N	2.71	0.49
1:A:1082:ARG:NH1	1:A:1082:ARG:CB	2.75	0.49
1:B:707:THR:O	1:B:707:THR:CG2	2.61	0.49
1:B:734:ARG:NH1	1:B:735:ASN:N	2.60	0.48
1:B:806:LEU:HD23	1:B:841:ILE:CD1	2.43	0.48
1:A:707:THR:O	1:A:707:THR:HG22	2.13	0.48
1:A:900:LEU:HD21	1:A:1200:ILE:HG22	1.95	0.48
1:A:993:ILE:HD13	1:A:1024:MSE:SE	2.62	0.48
1:B:932:TRP:CD2	1:B:933:ARG:HG3	2.48	0.48
1:B:1082:ARG:NH1	1:B:1082:ARG:CB	2.70	0.48
1:A:939:ASN:HA	1:A:944:LYS:HD3	1.95	0.48
1:B:813:VAL:HG21	1:B:838:TYR:HH	1.76	0.48
1:B:1025:ILE:HD11	1:B:1081:LEU:HD11	1.95	0.48
1:B:1034:VAL:HG12	1:B:1036:LEU:HD13	1.96	0.48
1:A:889:GLN:NE2	1:A:889:GLN:HA	2.28	0.48
1:A:1171:ASP:OD1	1:A:1174:GLN:HB2	2.14	0.48
1:A:1192:GLN:O	1:A:1195:PHE:HB3	2.13	0.48
1:B:910:ARG:HB2	1:B:915:GLU:O	2.12	0.48
1:A:707:THR:O	1:A:707:THR:CG2	2.60	0.48
1:A:1087:LYS:HE3	1:A:1087:LYS:CA	2.42	0.48
1:B:764:CYS:HB3	1:B:765:PRO:HD2	1.95	0.48
1:B:800:PRO:HD2	1:B:879:LEU:HD11	1.96	0.48
1:B:801:GLU:OE1	1:B:805:LEU:CD1	2.61	0.48
1:A:768:ILE:O	1:A:768:ILE:HG13	2.13	0.48
1:A:854:VAL:HG23	1:A:854:VAL:O	2.13	0.48
1:A:930:ARG:HH21	1:A:1184:LEU:HD21	1.78	0.48
1:A:897:LEU:CD1	1:A:1168:GLU:HA	2.44	0.48
1:B:1046:ILE:HG23	1:B:1145:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:ILE:HD11	1:A:1081:LEU:CD1	2.43	0.48
1:A:932:TRP:CD2	1:A:933:ARG:HG3	2.49	0.48
1:A:1001:TYR:CE1	1:A:1163:SER:HB3	2.49	0.48
1:A:1063:VAL:HG12	1:A:1081:LEU:CD2	2.44	0.48
1:A:1083:HIS:O	1:A:1085:LYS:N	2.47	0.48
1:B:844:MSE:HE2	1:B:856:VAL:HA	1.95	0.48
1:B:1045:GLU:HG3	1:B:1045:GLU:O	2.14	0.48
1:A:767:TYR:HA	1:A:790:GLN:O	2.14	0.48
1:A:1039:LEU:CD1	1:A:1049:GLN:HG3	2.43	0.48
1:A:863:LEU:C	1:A:865:ARG:N	2.72	0.47
1:B:839:ILE:HD12	1:B:870:MSE:HE1	1.95	0.47
1:B:929:TYR:CD2	1:B:1181:LYS:HG3	2.49	0.47
1:A:608:ILE:HD12	1:A:608:ILE:N	2.28	0.47
1:A:1191:GLU:CD	1:A:1191:GLU:H	2.22	0.47
1:B:922:GLU:HG2	1:B:1173:PHE:CD1	2.49	0.47
1:A:621:ILE:O	1:A:625:GLY:N	2.46	0.47
1:A:848:LEU:HD23	1:A:852:ASN:HA	1.96	0.47
1:A:958:ASN:O	1:A:959:ARG:O	2.32	0.47
1:B:611:ASP:OD1	1:B:612:ILE:HG23	2.15	0.47
1:B:1046:ILE:HG23	1:B:1145:ARG:HE	1.79	0.47
1:B:1131:GLY:O	1:B:1132:ASN:CB	2.62	0.47
1:A:609:HIS:O	1:A:610:ALA:C	2.57	0.47
1:A:660:ASP:C	1:A:661:ILE:HD12	2.38	0.47
1:A:929:TYR:OH	1:A:1177:LYS:HE2	2.15	0.47
1:A:1097:TYR:CD2	1:A:1112:LEU:HD23	2.48	0.47
1:B:657:ARG:NH2	1:B:737:CYS:HA	2.29	0.47
1:B:806:LEU:C	1:B:808:LYS:N	2.69	0.47
1:B:949:ASN:C	1:B:949:ASN:ND2	2.71	0.47
1:A:668:ARG:NH1	1:A:681:ASN:OD1	2.47	0.47
1:A:863:LEU:HB3	1:A:870:MSE:HG3	1.95	0.47
1:A:996:SER:OG	1:A:1183:ARG:NE	2.46	0.47
1:A:1160:LEU:O	1:A:1164:ALA:HB2	2.15	0.47
1:B:922:GLU:HA	1:B:925:ARG:HH21	1.79	0.47
1:B:1028:ARG:HD2	1:B:1028:ARG:N	2.30	0.47
1:B:1132:ASN:N	1:B:1132:ASN:ND2	2.63	0.47
1:A:602:LEU:HD22	1:A:602:LEU:N	2.18	0.47
1:A:1122:LYS:HB2	1:A:1122:LYS:HZ2	1.80	0.47
1:B:1055:LYS:O	1:B:1055:LYS:HG2	2.15	0.47
1:A:800:PRO:HD2	1:A:879:LEU:HD11	1.96	0.46
1:A:962:LEU:HD12	1:A:993:ILE:HB	1.96	0.46
1:A:1000:SER:HB3	1:A:1005:GLU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:LEU:O	1:A:1165:GLU:HG2	2.14	0.46
1:B:1040:LYS:HA	1:B:1046:ILE:HG13	1.97	0.46
1:A:734:ARG:CZ	1:A:734:ARG:HA	2.45	0.46
1:A:896:ASN:ND2	1:A:1169:VAL:HG23	2.30	0.46
1:A:925:ARG:HE	1:A:925:ARG:HB2	1.61	0.46
1:A:618:LYS:O	1:A:621:ILE:HG13	2.15	0.46
1:A:657:ARG:NH1	1:A:703:PRO:O	2.45	0.46
1:B:689:ASP:N	1:B:866:GLN:HE22	2.13	0.46
1:A:844:MSE:HE2	1:A:856:VAL:HA	1.97	0.46
1:A:922:GLU:HG2	1:A:1173:PHE:CD1	2.50	0.46
1:B:708:VAL:HG23	1:B:709:ASP:N	2.30	0.46
1:B:767:TYR:HA	1:B:790:GLN:O	2.15	0.46
1:A:646:GLU:HG3	1:A:668:ARG:NH2	2.30	0.46
1:A:775:VAL:HG12	1:A:783:GLY:HA3	1.97	0.46
1:A:1061:ILE:HD12	1:A:1061:ILE:O	2.15	0.46
1:B:764:CYS:HB3	1:B:765:PRO:CD	2.45	0.46
1:B:938:GLY:HA3	1:B:953:ILE:CG2	2.46	0.46
1:A:839:ILE:HD12	1:A:870:MSE:HE1	1.97	0.46
1:A:940:GLN:OE1	1:A:940:GLN:CA	2.55	0.46
1:A:1064:ASP:OD2	1:A:1066:LYS:HE2	2.16	0.46
1:B:668:ARG:NH1	1:B:681:ASN:OD1	2.49	0.46
1:B:831:GLY:O	1:B:867:ARG:HD3	2.15	0.46
1:A:958:ASN:N	1:A:958:ASN:HD22	2.13	0.46
1:A:1170:VAL:HG12	1:A:1172:ILE:HG13	1.98	0.46
1:B:614:LEU:HG	1:B:889:GLN:HE22	1.79	0.46
1:B:618:LYS:HA	1:B:621:ILE:HD11	1.98	0.46
1:A:831:GLY:C	1:A:835:THR:HG21	2.41	0.46
1:A:1020:ASP:HA	1:A:1023:GLN:OE1	2.16	0.46
1:B:615:GLU:OE2	1:B:615:GLU:N	2.41	0.46
1:B:1112:LEU:O	1:B:1116:ILE:HG13	2.16	0.46
1:B:1070:LYS:HG2	1:B:1075:THR:CG2	2.46	0.46
1:B:806:LEU:C	1:B:808:LYS:H	2.24	0.45
1:B:904:LEU:HD13	1:B:1197:TYR:CD1	2.51	0.45
1:B:864:ARG:HH11	1:B:864:ARG:CG	2.23	0.45
1:B:918:PRO:O	1:B:921:ALA:HB3	2.16	0.45
1:A:901:HIS:CB	1:A:902:PRO:HD3	2.46	0.45
1:A:1025:ILE:HD12	1:A:1025:ILE:O	2.16	0.45
1:B:673:GLU:HG2	1:B:681:ASN:HB3	1.98	0.45
1:B:1041:HIS:O	1:B:1043:ASP:N	2.49	0.45
1:A:1017:THR:C	1:A:1019:GLY:H	2.24	0.45
1:A:1153:ILE:HD11	1:A:1192:GLN:CB	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:ARG:HG3	1:B:1089:SER:HA	1.99	0.45
1:B:1160:LEU:HD21	1:B:1172:ILE:HA	1.98	0.45
1:A:741:TRP:HB2	1:A:742:PRO:HD2	1.97	0.45
1:A:1045:GLU:HG3	1:A:1045:GLU:O	2.16	0.45
1:A:1097:TYR:CD1	1:A:1115:MSE:HG3	2.52	0.45
1:B:863:LEU:C	1:B:865:ARG:N	2.73	0.45
1:B:1022:TRP:CZ2	1:B:1050:TYR:HD1	2.34	0.45
1:B:1026:PHE:CE2	1:B:1090:ARG:NH1	2.85	0.45
1:B:1097:TYR:CE2	1:B:1112:LEU:HD23	2.51	0.45
1:A:1022:TRP:CZ2	1:A:1050:TYR:HD1	2.35	0.45
1:B:605:VAL:HG21	1:B:857:TYR:HB2	1.97	0.45
1:B:832:VAL:HG23	1:B:833:GLY:N	2.31	0.45
1:B:1083:HIS:O	1:B:1085:LYS:N	2.49	0.45
1:A:864:ARG:HD2	1:A:870:MSE:H	1.81	0.45
1:A:1061:ILE:C	1:A:1061:ILE:CD1	2.89	0.45
1:B:608:ILE:O	1:B:853:LYS:HA	2.17	0.45
1:B:880:ILE:O	1:B:883:ALA:HB3	2.17	0.45
1:A:1107:ALA:C	1:A:1109:PRO:HD3	2.42	0.45
1:B:641:LYS:O	1:B:643:PRO:HD3	2.17	0.45
1:B:1170:VAL:HG12	1:B:1172:ILE:HG13	1.98	0.45
2:C:2004:PTR:O	2:C:2005:SER:HB2	2.16	0.45
1:A:643:PRO:O	1:A:665:ASP:HB2	2.17	0.45
1:A:756:VAL:HG22	1:A:774:ILE:HG22	1.99	0.45
1:A:938:GLY:HA3	1:A:953:ILE:HG21	1.99	0.45
1:B:859:TYR:CE1	1:B:863:LEU:HD11	2.52	0.45
1:B:1014:LEU:HB3	1:B:1016:GLU:HG2	1.98	0.45
1:B:1017:THR:C	1:B:1019:GLY:H	2.24	0.45
1:A:618:LYS:HA	1:A:621:ILE:HD11	1.99	0.45
1:A:922:GLU:HA	1:A:925:ARG:HH21	1.82	0.45
1:A:1019:GLY:C	1:A:1023:GLN:OE1	2.60	0.44
1:A:1026:PHE:HA	1:A:1090:ARG:NH2	2.32	0.44
1:A:1041:HIS:O	1:A:1043:ASP:N	2.49	0.44
1:B:859:TYR:O	1:B:863:LEU:HG	2.17	0.44
1:B:926:LEU:HD11	1:B:1193:TYR:HE1	1.78	0.44
1:A:807:LEU:HD21	1:A:887:TYR:HB2	1.98	0.44
1:A:811:ARG:NH1	1:A:892:GLU:OE2	2.48	0.44
1:B:779:GLU:O	1:B:781:ALA:N	2.50	0.44
1:B:947:ASN:CG	1:B:994:ASN:HD22	2.24	0.44
1:B:1051:TRP:HB2	1:B:1079:PHE:HE2	1.82	0.44
1:B:1114:SER:HA	1:B:1117:GLN:CG	2.46	0.44
1:B:1153:ILE:HD13	1:B:1187:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:LEU:HD13	1:A:1197:TYR:CD1	2.52	0.44
1:A:910:ARG:HB3	1:A:917:SER:CB	2.47	0.44
1:B:930:ARG:HH21	1:B:1184:LEU:HD11	1.81	0.44
1:B:1085:LYS:O	1:B:1085:LYS:HG2	2.17	0.44
1:B:1107:ALA:C	1:B:1109:PRO:HD3	2.42	0.44
1:A:841:ILE:O	1:A:845:LEU:HG	2.17	0.44
1:A:948:ARG:NH2	1:A:1047:CYS:HA	2.33	0.44
1:A:1026:PHE:HA	1:A:1090:ARG:HH22	1.83	0.44
1:A:1179:LEU:O	1:A:1180:ARG:C	2.59	0.44
1:B:831:GLY:CA	1:B:835:THR:HG21	2.47	0.44
1:B:1187:VAL:HA	1:B:1192:GLN:OE1	2.17	0.44
1:A:644:ILE:HG12	1:A:664:TYR:HA	2.00	0.44
1:A:661:ILE:N	1:A:661:ILE:CD1	2.80	0.44
1:A:1172:ILE:HD12	1:A:1197:TYR:CE1	2.53	0.44
1:B:869:LEU:O	1:B:869:LEU:HG	2.18	0.44
1:A:687:TYR:CG	1:A:695:ARG:HD2	2.53	0.44
1:A:831:GLY:O	1:A:867:ARG:HD3	2.17	0.44
1:A:922:GLU:HG2	1:A:1173:PHE:HD1	1.83	0.44
1:A:1082:ARG:HD2	1:A:1086:ARG:HA	1.98	0.44
1:B:813:VAL:HA	1:B:816:PHE:CD2	2.52	0.44
1:B:1097:TYR:CD1	1:B:1115:MSE:HG3	2.53	0.44
1:A:845:LEU:HD23	1:A:884:LEU:HD23	2.00	0.44
1:A:903:TYR:O	1:A:904:LEU:C	2.60	0.44
1:A:1060:ASP:O	1:A:1083:HIS:CB	2.66	0.44
1:B:614:LEU:CD2	1:B:889:GLN:NE2	2.81	0.44
1:B:631:GLU:HG2	1:B:877:TYR:OH	2.18	0.44
1:B:910:ARG:O	1:B:911:ASP:C	2.60	0.44
1:B:922:GLU:HG2	1:B:1173:PHE:HD1	1.83	0.44
1:B:1126:LYS:HB3	1:B:1126:LYS:HZ3	1.82	0.44
1:A:784:ARG:HD2	1:A:820:PHE:CZ	2.53	0.44
1:A:1141:LEU:HD23	1:A:1141:LEU:C	2.43	0.44
1:B:806:LEU:HA	1:B:806:LEU:HD12	1.66	0.44
1:B:806:LEU:O	1:B:809:LEU:HD23	2.18	0.44
1:A:1101:SER:HB3	1:A:1103:GLU:OE1	2.18	0.44
1:B:789:ILE:HG12	1:B:816:PHE:HE2	1.82	0.44
1:B:958:ASN:N	1:B:958:ASN:HD22	2.16	0.44
1:A:832:VAL:HG23	1:A:833:GLY:N	2.33	0.43
1:A:1055:LYS:O	1:A:1056:GLN:C	2.60	0.43
1:A:1076:LEU:O	1:A:1076:LEU:HG	2.17	0.43
1:B:677:ASP:CG	1:B:680:SER:HB3	2.43	0.43
1:B:912:PRO:HA	1:B:913:PRO:HD2	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1029:LYS:HA	1:B:1090:ARG:NH2	2.33	0.43
1:B:1060:ASP:O	1:B:1083:HIS:CB	2.66	0.43
1:A:689:ASP:N	1:A:866:GLN:HE22	2.17	0.43
1:A:804:HIS:O	1:A:808:LYS:HB2	2.17	0.43
1:B:661:ILE:O	1:B:662:LEU:HD23	2.18	0.43
1:B:748:THR:OG1	1:B:757:LYS:HG3	2.18	0.43
1:A:1044:GLN:HE21	1:A:1044:GLN:N	2.16	0.43
1:B:650:PRO:C	1:B:652:ASN:H	2.26	0.43
1:B:716:TRP:CE2	1:B:776:ASN:HB2	2.53	0.43
1:B:863:LEU:HB3	1:B:870:MSE:HG3	1.99	0.43
1:A:631:GLU:O	1:A:857:TYR:CE1	2.69	0.43
1:A:1070:LYS:HG2	1:A:1075:THR:CB	2.46	0.43
1:B:715:ILE:CD1	1:B:825:VAL:HG21	2.48	0.43
1:B:832:VAL:HG12	1:B:867:ARG:HG2	1.98	0.43
1:A:802:ASP:OD2	1:A:804:HIS:HB3	2.18	0.43
1:A:1055:LYS:O	1:A:1055:LYS:HG2	2.18	0.43
1:A:1123:LEU:HA	1:A:1124:PRO:HD3	1.78	0.43
1:A:697:TYR:CE1	1:A:839:ILE:HG23	2.53	0.43
1:A:813:VAL:C	1:A:815:ALA:N	2.76	0.43
1:A:873:VAL:CG1	1:A:875:ALA:H	2.20	0.43
1:A:1051:TRP:HB2	1:A:1079:PHE:HE2	1.82	0.43
1:A:1153:ILE:HD11	1:A:1192:GLN:CD	2.44	0.43
1:B:802:ASP:OD2	1:B:804:HIS:HB3	2.19	0.43
1:B:806:LEU:HD12	1:B:809:LEU:CD2	2.49	0.43
1:A:691:PHE:O	1:A:692:LYS:HG2	2.19	0.43
1:A:831:GLY:CA	1:A:835:THR:HG21	2.49	0.43
1:B:1028:ARG:HG3	1:B:1028:ARG:NH1	2.34	0.43
1:B:1049:GLN:C	1:B:1051:TRP:N	2.77	0.43
1:B:1191:GLU:CD	1:B:1191:GLU:H	2.27	0.43
1:A:1046:ILE:CG2	1:A:1145:ARG:HG2	2.49	0.43
1:A:1082:ARG:HG3	1:A:1089:SER:HA	2.00	0.43
1:B:1026:PHE:HA	1:B:1090:ARG:HH22	1.84	0.43
1:A:896:ASN:N	1:A:896:ASN:HD22	2.15	0.43
1:B:614:LEU:HD22	1:B:885:VAL:HG13	2.01	0.43
1:B:614:LEU:HD21	1:B:889:GLN:CD	2.43	0.43
1:B:1064:ASP:OD2	1:B:1066:LYS:HE2	2.19	0.43
1:B:1109:PRO:O	1:B:1110:LYS:C	2.60	0.43
1:A:599:GLU:CB	1:A:865:ARG:NH2	2.81	0.43
1:A:806:LEU:O	1:A:809:LEU:HD23	2.19	0.43
1:A:1039:LEU:HD23	1:A:1039:LEU:HA	1.87	0.43
1:A:1083:HIS:C	1:A:1085:LYS:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:801:GLU:HG2	1:B:1003:LYS:HE3	2.01	0.42
1:B:841:ILE:O	1:B:845:LEU:HG	2.19	0.42
1:B:1010:ALA:O	1:B:1147:GLY:HA3	2.19	0.42
1:B:1109:PRO:O	1:B:1112:LEU:N	2.50	0.42
1:B:777:LYS:HD3	1:B:777:LYS:HA	1.76	0.42
1:B:813:VAL:C	1:B:815:ALA:N	2.74	0.42
1:B:962:LEU:HG	1:B:993:ILE:HG22	2.01	0.42
1:B:1061:ILE:C	1:B:1061:ILE:CD1	2.87	0.42
1:B:804:HIS:O	1:B:808:LYS:HB2	2.18	0.42
1:B:908:LYS:O	1:B:909:LYS:C	2.62	0.42
1:B:927:PRO:O	1:B:928:SER:C	2.63	0.42
1:A:789:ILE:HG12	1:A:816:PHE:CE2	2.53	0.42
1:A:806:LEU:C	1:A:808:LYS:H	2.27	0.42
1:B:708:VAL:HG23	1:B:709:ASP:H	1.84	0.42
1:A:753:ASP:OD1	1:A:778:LYS:HD3	2.19	0.42
1:B:625:GLY:C	1:B:627:PRO:HD2	2.44	0.42
1:B:667:ASN:O	1:B:687:TYR:HD1	2.03	0.42
1:B:993:ILE:O	1:B:995:ALA:N	2.49	0.42
1:B:1011:GLN:HA	1:B:1144:CYS:O	2.20	0.42
1:B:1018:ILE:HD11	1:B:1049:GLN:H	1.84	0.42
1:B:1040:LYS:HA	1:B:1046:ILE:H	1.85	0.42
1:B:1001:TYR:CE1	1:B:1163:SER:HB3	2.54	0.42
1:B:1007:MSE:SE	1:B:1158:LEU:HD12	2.70	0.42
1:A:828:SER:OG	1:A:835:THR:HG22	2.18	0.42
1:A:1028:ARG:HG3	1:A:1028:ARG:HH11	1.84	0.42
1:A:1083:HIS:NE2	1:A:1085:LYS:HE2	2.35	0.42
1:B:660:ASP:OD2	2:D:2005:SER:N	2.53	0.42
1:B:1039:LEU:CD2	1:B:1048:ALA:O	2.67	0.42
1:B:1039:LEU:CD1	1:B:1049:GLN:HG3	2.48	0.42
1:B:1076:LEU:O	1:B:1076:LEU:HG	2.20	0.42
1:A:736:LYS:HA	1:A:736:LYS:HD3	1.89	0.42
1:A:952:VAL:HG12	1:A:1183:ARG:HH12	1.84	0.42
1:B:1044:GLN:H	1:B:1044:GLN:CD	2.25	0.42
1:A:599:GLU:N	1:A:641:LYS:HE2	2.35	0.42
1:A:1114:SER:HA	1:A:1117:GLN:CG	2.50	0.42
1:B:876:GLN:O	1:B:880:ILE:HG13	2.20	0.42
1:B:907:MSE:HE2	1:B:922:GLU:OE1	2.20	0.42
1:B:939:ASN:HA	1:B:944:LYS:HD3	2.00	0.42
1:B:1148:SER:OG	1:B:1183:ARG:HD3	2.20	0.42
1:A:614:LEU:HD22	1:A:885:VAL:HG13	2.01	0.42
1:B:657:ARG:HH12	1:B:704:ARG:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:ASP:CB	1:B:912:PRO:CD	2.94	0.42
1:B:1153:ILE:HD11	1:B:1192:GLN:CB	2.37	0.42
1:A:902:PRO:O	1:A:905:HIS:HB3	2.20	0.41
1:A:963:LYS:CE	1:A:1027:GLN:HB3	2.46	0.41
1:A:1167:GLU:O	1:A:1168:GLU:HB2	2.20	0.41
1:A:761:HIS:HE1	1:A:763:ARG:CZ	2.34	0.41
1:A:932:TRP:CH2	1:A:933:ARG:NE	2.88	0.41
1:A:954:PRO:HD3	1:A:994:ASN:OD1	2.20	0.41
1:A:1034:VAL:HG12	1:A:1036:LEU:HD13	2.02	0.41
1:B:723:ILE:O	1:B:789:ILE:HD12	2.20	0.41
1:B:854:VAL:O	1:B:854:VAL:HG23	2.20	0.41
1:B:864:ARG:HD2	1:B:870:MSE:HB2	2.02	0.41
1:B:951:ASN:C	1:B:951:ASN:HD22	2.27	0.41
1:A:806:LEU:HA	1:A:809:LEU:CD2	2.50	0.41
1:A:930:ARG:CG	1:A:931:SER:N	2.83	0.41
1:A:1019:GLY:O	1:A:1023:GLN:OE1	2.37	0.41
1:B:811:ARG:HD2	1:B:892:GLU:HG3	2.02	0.41
1:B:1128:SER:O	1:B:1129:SER:CB	2.67	0.41
1:A:650:PRO:C	1:A:652:ASN:H	2.28	0.41
1:A:708:VAL:HG23	1:A:709:ASP:N	2.35	0.41
1:A:789:ILE:CG1	1:A:816:PHE:CE2	2.98	0.41
1:A:813:VAL:HG21	1:A:838:TYR:HH	1.80	0.41
1:A:890:PHE:HE2	1:A:927:PRO:HD3	1.81	0.41
1:A:1028:ARG:N	1:A:1028:ARG:HD2	2.34	0.41
1:B:726:VAL:O	1:B:727:THR:HB	2.19	0.41
1:B:1153:ILE:HD11	1:B:1192:GLN:CD	2.45	0.41
1:A:951:ASN:C	1:A:951:ASN:HD22	2.28	0.41
1:B:801:GLU:OE1	1:B:805:LEU:HD11	2.21	0.41
1:B:911:ASP:O	1:B:912:PRO:C	2.64	0.41
1:A:832:VAL:HG12	1:A:867:ARG:HG2	2.02	0.41
1:A:863:LEU:HD22	1:A:870:MSE:HE2	2.02	0.41
1:A:887:TYR:O	1:A:891:GLY:HA2	2.21	0.41
1:A:894:GLU:HG2	1:A:1169:VAL:HG22	2.03	0.41
1:B:728:ARG:HH21	1:B:792:THR:HB	1.85	0.41
1:B:1006:VAL:HG12	1:B:1007:MSE:N	2.34	0.41
1:A:726:VAL:O	1:A:727:THR:HB	2.21	0.41
1:A:1015:LYS:HB3	1:A:1015:LYS:HZ3	1.86	0.41
1:A:1049:GLN:C	1:A:1051:TRP:N	2.79	0.41
1:A:1111:GLU:HA	1:A:1114:SER:OG	2.21	0.41
1:B:624:GLU:OE2	1:B:624:GLU:O	2.39	0.41
1:B:1083:HIS:C	1:B:1085:LYS:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1123:LEU:HB2	1:B:1124:PRO:CD	2.51	0.41
1:B:1180:ARG:HH11	1:B:1180:ARG:HG2	1.86	0.41
1:A:906:ASN:O	1:A:909:LYS:HG3	2.21	0.41
1:A:1013:PRO:HD2	1:A:1047:CYS:SG	2.61	0.41
1:B:908:LYS:O	1:B:917:SER:CB	2.68	0.41
1:B:1133:LYS:HG3	1:B:1134:HIS:N	2.35	0.41
1:A:659:VAL:HG22	1:A:659:VAL:O	2.22	0.40
1:A:936:HIS:N	1:A:956:ASP:OD2	2.47	0.40
1:A:960:VAL:HG23	1:A:995:ALA:O	2.22	0.40
1:B:608:ILE:HG21	1:B:613:LEU:HA	2.02	0.40
1:B:734:ARG:HH11	1:B:734:ARG:HB3	1.86	0.40
1:B:807:LEU:HD21	1:B:887:TYR:HB2	2.01	0.40
1:B:845:LEU:HD23	1:B:884:LEU:HD23	2.03	0.40
1:B:934:THR:OG1	1:B:956:ASP:HB2	2.21	0.40
1:B:958:ASN:O	1:B:959:ARG:C	2.63	0.40
1:B:1034:VAL:HG12	1:B:1036:LEU:CD1	2.52	0.40
1:A:661:ILE:O	1:A:662:LEU:HD23	2.22	0.40
1:A:716:TRP:CE2	1:A:776:ASN:HB2	2.56	0.40
1:A:932:TRP:CZ2	1:A:1181:LYS:HG2	2.57	0.40
1:B:651:PHE:O	1:B:655:LYS:HE3	2.21	0.40
1:A:1060:ASP:O	1:A:1083:HIS:HB3	2.21	0.40
1:A:1110:LYS:HG2	1:A:1111:GLU:N	2.37	0.40
1:B:873:VAL:O	1:B:877:TYR:N	2.49	0.40
1:B:1122:LYS:HB2	1:B:1122:LYS:HZ2	1.85	0.40
1:A:1018:ILE:HD11	1:A:1049:GLN:H	1.85	0.40
1:A:1025:ILE:HD11	1:A:1081:LEU:HD11	2.02	0.40
1:A:1046:ILE:HG23	1:A:1145:ARG:CG	2.50	0.40
1:B:643:PRO:O	1:B:665:ASP:HB2	2.21	0.40
1:B:938:GLY:HA2	1:B:992:TYR:CZ	2.56	0.40
1:B:991:LYS:HD3	1:B:991:LYS:N	2.36	0.40

There are no symmetry-related clashes.

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	565/610 (93%)	461 (82%)	80 (14%)	24 (4%)	2	9
1	B	578/610 (95%)	451 (78%)	93 (16%)	34 (6%)	1	4
2	C	1/4 (25%)	1 (100%)	0	0	100	100
2	D	1/4 (25%)	1 (100%)	0	0	100	100
All	All	1145/1228 (93%)	914 (80%)	173 (15%)	58 (5%)	1	6

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	819	PHE
1	A	870	MSE
1	A	871	VAL
1	A	911	ASP
1	A	930	ARG
1	A	1050	TYR
1	A	1086	ARG
1	A	1099	ASN
1	A	1187	VAL
1	B	870	MSE
1	B	871	VAL
1	B	895	VAL
1	B	911	ASP
1	B	930	ARG
1	B	1050	TYR
1	B	1086	ARG
1	B	1099	ASN
1	B	1123	LEU
1	B	1124	PRO
1	B	1129	SER
1	B	1132	ASN
1	B	1133	LYS
1	B	1186	MSE
1	A	610	ALA
1	A	833	GLY
1	A	1042	GLY
1	A	1056	GLN
1	A	1084	SER
1	B	833	GLY
1	B	941	GLU

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Mol	Chain	Res	Type
1	B	1042	GLY
1	B	1056	GLN
1	B	1084	SER
1	B	1145	ARG
1	A	932	TRP
1	A	941	GLU
1	A	959	ARG
1	A	1015	LYS
1	A	1089	SER
1	A	1145	ARG
1	B	610	ALA
1	B	780	LYS
1	B	932	TRP
1	B	1018	ILE
1	B	1048	ALA
1	B	1089	SER
1	A	1018	ILE
1	B	915	GLU
1	B	991	LYS
1	B	1015	LYS
1	B	1149	GLN
1	A	1048	ALA
1	B	1102	VAL
1	A	903	TYR
1	A	1102	VAL
1	B	913	PRO
1	B	747	GLY
1	B	1138	THR

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	514/538 (96%)	450 (88%)	64 (12%)	4	15
1	B	524/538 (97%)	456 (87%)	68 (13%)	4	13
2	C	3/3 (100%)	2 (67%)	1 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	1044/1082 (96%)	911 (87%)	133 (13%)	4	14

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	602	LEU
1	A	611	ASP
1	A	614	LEU
1	A	621	ILE
1	A	629	LEU
1	A	637	ARG
1	A	641	LYS
1	A	665	ASP
1	A	701	GLN
1	A	721	THR
1	A	734	ARG
1	A	775	VAL
1	A	782	THR
1	A	785	GLU
1	A	789	ILE
1	A	792	THR
1	A	806	LEU
1	A	835	THR
1	A	848	LEU
1	A	864	ARG
1	A	872	GLN
1	A	874	GLU
1	A	879	LEU
1	A	909	LYS
1	A	910	ARG
1	A	911	ASP
1	A	919	LEU
1	A	925	ARG
1	A	940	GLN
1	A	951	ASN
1	A	957	TYR
1	A	958	ASN
1	A	963	LYS
1	A	991	LYS
1	A	996	SER
1	A	1015	LYS

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Mol	Chain	Res	Type
1	A	1016	GLU
1	A	1025	ILE
1	A	1028	ARG
1	A	1036	LEU
1	A	1043	ASP
1	A	1044	GLN
1	A	1049	GLN
1	A	1061	ILE
1	A	1065	LEU
1	A	1075	THR
1	A	1076	LEU
1	A	1082	ARG
1	A	1083	HIS
1	A	1087	LYS
1	A	1091	THR
1	A	1104	GLN
1	A	1114	SER
1	A	1115	MSE
1	A	1118	VAL
1	A	1120	LYS
1	A	1121	GLN
1	A	1122	LYS
1	A	1125	GLN
1	A	1150	GLN
1	A	1169	VAL
1	A	1180	ARG
1	A	1184	LEU
1	A	1186	MSE
1	B	602	LEU
1	B	611	ASP
1	B	614	LEU
1	B	621	ILE
1	B	629	LEU
1	B	637	ARG
1	B	641	LYS
1	B	665	ASP
1	B	701	GLN
1	B	721	THR
1	B	734	ARG
1	B	775	VAL
1	B	778	LYS
1	B	782	THR

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Mol	Chain	Res	Type
1	B	785	GLU
1	B	789	ILE
1	B	792	THR
1	B	806	LEU
1	B	820	PHE
1	B	835	THR
1	B	848	LEU
1	B	864	ARG
1	B	872	GLN
1	B	874	GLU
1	B	879	LEU
1	B	888	ASN
1	B	896	ASN
1	B	909	LYS
1	B	919	LEU
1	B	925	ARG
1	B	940	GLN
1	B	951	ASN
1	B	957	TYR
1	B	958	ASN
1	B	991	LYS
1	B	992	TYR
1	B	996	SER
1	B	999	MSE
1	B	1015	LYS
1	B	1016	GLU
1	B	1018	ILE
1	B	1025	ILE
1	B	1028	ARG
1	B	1036	LEU
1	B	1043	ASP
1	B	1044	GLN
1	B	1049	GLN
1	B	1065	LEU
1	B	1075	THR
1	B	1076	LEU
1	B	1082	ARG
1	B	1083	HIS
1	B	1087	LYS
1	B	1091	THR
1	B	1104	GLN
1	B	1114	SER

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Mol	Chain	Res	Type
1	B	1120	LYS
1	B	1121	GLN
1	B	1122	LYS
1	B	1124	PRO
1	B	1126	LYS
1	B	1128	SER
1	B	1130	GLU
1	B	1132	ASN
1	B	1150	GLN
1	B	1169	VAL
1	B	1180	ARG
1	B	1184	LEU
2	C	2003	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	604	ASN
1	A	633	GLN
1	A	652	ASN
1	A	653	GLN
1	A	718	GLN
1	A	761	HIS
1	A	770	GLN
1	A	866	GLN
1	A	882	GLN
1	A	889	GLN
1	A	896	ASN
1	A	924	GLN
1	A	936	HIS
1	A	943	ASN
1	A	947	ASN
1	A	949	ASN
1	A	951	ASN
1	A	958	ASN
1	A	1027	GLN
1	A	1044	GLN
1	A	1049	GLN
1	A	1094	GLN
1	A	1117	GLN
1	A	1121	GLN
1	A	1149	GLN

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Mol	Chain	Res	Type
1	A	1194	GLN
1	B	604	ASN
1	B	633	GLN
1	B	652	ASN
1	B	718	GLN
1	B	761	HIS
1	B	770	GLN
1	B	866	GLN
1	B	882	GLN
1	B	889	GLN
1	B	906	ASN
1	B	924	GLN
1	B	943	ASN
1	B	947	ASN
1	B	949	ASN
1	B	951	ASN
1	B	958	ASN
1	B	994	ASN
1	B	1027	GLN
1	B	1044	GLN
1	B	1049	GLN
1	B	1094	GLN
1	B	1117	GLN
1	B	1121	GLN
1	B	1125	GLN
1	B	1132	ASN
1	B	1134	HIS
1	B	1149	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PTR	D	2004	2	15,16,17	1.81	5 (33%)	17,22,24	2.41	6 (35%)
2	PTR	C	2004	2	15,16,17	1.76	5 (33%)	17,22,24	1.96	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	D	2004	2	1/1/2/3	3/10/11/13	0/1/1/1
2	PTR	C	2004	2	1/1/2/3	3/10/11/13	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2004	PTR	P-OH	3.32	1.65	1.59
2	C	2004	PTR	P-OH	2.93	1.65	1.59
2	C	2004	PTR	OH-CZ	2.89	1.47	1.40
2	D	2004	PTR	OH-CZ	2.88	1.47	1.40
2	C	2004	PTR	P-O3P	-2.70	1.44	1.54
2	D	2004	PTR	P-O3P	-2.65	1.45	1.54
2	C	2004	PTR	CE2-CD2	2.55	1.42	1.38
2	D	2004	PTR	CE2-CD2	2.49	1.42	1.38
2	D	2004	PTR	CD2-CG	2.37	1.43	1.38
2	C	2004	PTR	CD2-CG	2.32	1.43	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2004	PTR	OH-CZ-CE2	5.76	136.48	119.22
2	D	2004	PTR	OH-CZ-CE1	-5.54	102.61	119.22
2	C	2004	PTR	OH-CZ-CE2	4.58	132.95	119.22
2	C	2004	PTR	OH-CZ-CE1	-4.26	106.43	119.22
2	D	2004	PTR	P-OH-CZ	2.76	133.71	123.88
2	D	2004	PTR	CE2-CD2-CG	-2.39	117.85	121.00
2	D	2004	PTR	CB-CG-CD1	-2.39	116.46	120.90
2	C	2004	PTR	CE2-CD2-CG	-2.21	118.10	121.00
2	D	2004	PTR	O3P-P-O2P	2.15	115.85	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2004	PTR	CB-CG-CD1	-2.14	116.92	120.90
2	C	2004	PTR	O3P-P-OH	2.12	111.59	105.32

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2004	PTR	CA
2	D	2004	PTR	CA

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2004	PTR	C-CA-CB-CG
2	D	2004	PTR	C-CA-CB-CG
2	D	2004	PTR	CA-CB-CG-CD2
2	D	2004	PTR	CA-CB-CG-CD1
2	C	2004	PTR	CA-CB-CG-CD2
2	C	2004	PTR	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2004	PTR	1	0

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.