



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:07 AM UTC

PDB ID : 2QCJ / pdb_00002qcj
Title : Native Structure of Lyp
Authors : Sun, J.P.; Yu, X.; Zhang, Z.Y.
Deposited on : 2007-06-19
Resolution : 3.00 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

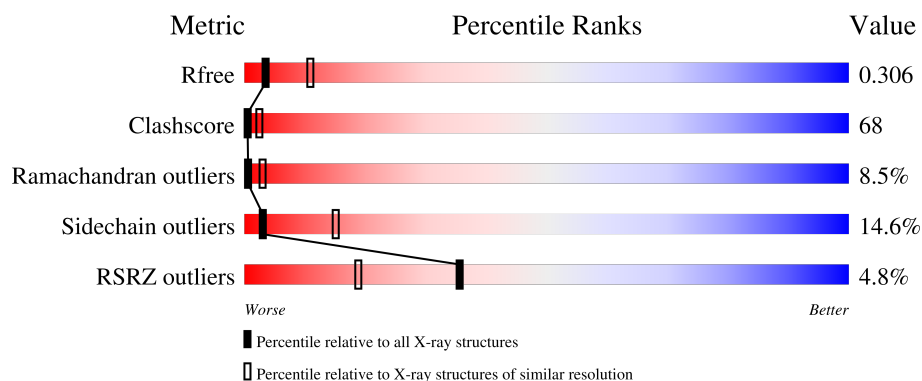
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	313	
1	B	313	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4631 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 Tyrosine-protein phosphatase non-receptor type 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2304	1488	374	427	15			
1	B	280	Total	C	N	O	S	0	0	0
			2304	1488	374	427	15			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	HIS	-	expression tag	UNP Q9Y2R2
A	-17	HIS	-	expression tag	UNP Q9Y2R2
A	-16	HIS	-	expression tag	UNP Q9Y2R2
A	-15	HIS	-	expression tag	UNP Q9Y2R2
A	-14	HIS	-	expression tag	UNP Q9Y2R2
A	-13	HIS	-	expression tag	UNP Q9Y2R2
A	-12	SER	-	expression tag	UNP Q9Y2R2
A	-11	SER	-	expression tag	UNP Q9Y2R2
A	-10	GLY	-	expression tag	UNP Q9Y2R2
A	-9	LEU	-	expression tag	UNP Q9Y2R2
A	-8	VAL	-	expression tag	UNP Q9Y2R2
A	-7	PRO	-	expression tag	UNP Q9Y2R2
A	-6	ARG	-	expression tag	UNP Q9Y2R2
A	-5	GLY	-	expression tag	UNP Q9Y2R2
A	-4	SER	-	expression tag	UNP Q9Y2R2
A	-3	HIS	-	expression tag	UNP Q9Y2R2
A	-2	MET	-	expression tag	UNP Q9Y2R2
A	-1	ALA	-	expression tag	UNP Q9Y2R2
A	0	SER	-	expression tag	UNP Q9Y2R2
B	-18	HIS	-	expression tag	UNP Q9Y2R2
B	-17	HIS	-	expression tag	UNP Q9Y2R2
B	-16	HIS	-	expression tag	UNP Q9Y2R2
B	-15	HIS	-	expression tag	UNP Q9Y2R2
B	-14	HIS	-	expression tag	UNP Q9Y2R2
B	-13	HIS	-	expression tag	UNP Q9Y2R2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	SER	-	expression tag	UNP Q9Y2R2
B	-11	SER	-	expression tag	UNP Q9Y2R2
B	-10	GLY	-	expression tag	UNP Q9Y2R2
B	-9	LEU	-	expression tag	UNP Q9Y2R2
B	-8	VAL	-	expression tag	UNP Q9Y2R2
B	-7	PRO	-	expression tag	UNP Q9Y2R2
B	-6	ARG	-	expression tag	UNP Q9Y2R2
B	-5	GLY	-	expression tag	UNP Q9Y2R2
B	-4	SER	-	expression tag	UNP Q9Y2R2
B	-3	HIS	-	expression tag	UNP Q9Y2R2
B	-2	MET	-	expression tag	UNP Q9Y2R2
B	-1	ALA	-	expression tag	UNP Q9Y2R2
B	0	SER	-	expression tag	UNP Q9Y2R2

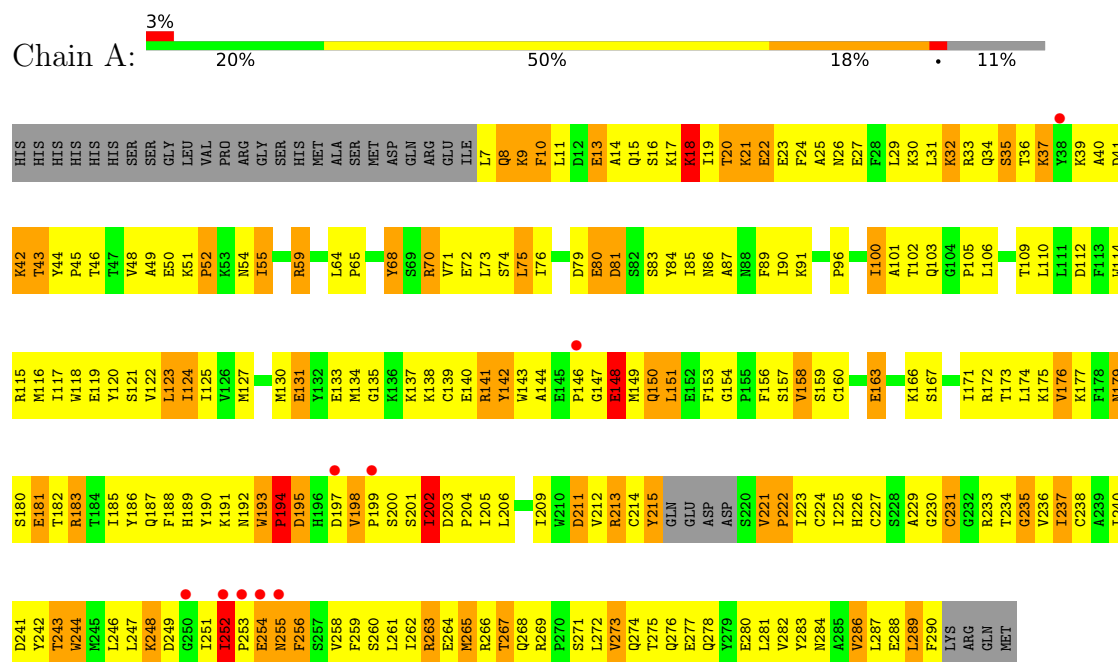
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	11	Total O 11 11	0	0

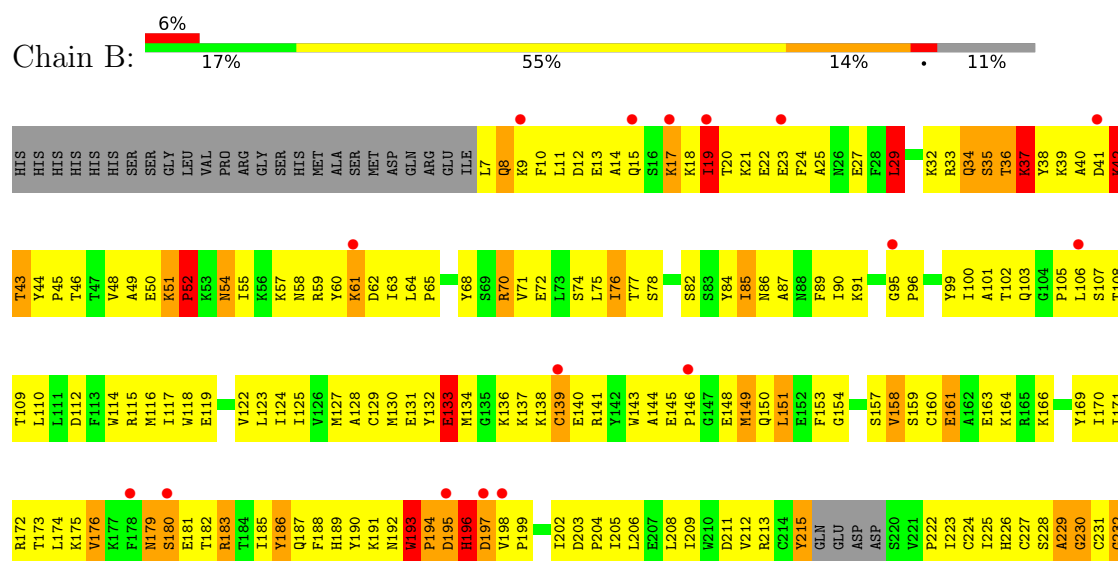
3 Residue-property plots

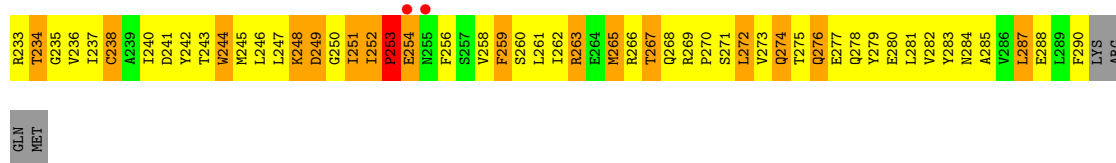
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Tyrosine-protein phosphatase non-receptor type 22



- Molecule 1: Tyrosine-protein phosphatase non-receptor type 22





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.31Å 93.95Å 148.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.2 (50.00-3.00) 92.1 (50.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.284 , 0.307 0.284 , 0.306	Depositor DCC
R_{free} test set	990 reflections (6.11%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 108.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4631	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9045e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.55	0/2360	1.16	19/3191 (0.6%)
1	B	0.59	0/2360	1.12	20/3191 (0.6%)
All	All	0.57	0/4720	1.14	39/6382 (0.6%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	LEU	N-CA-C	-13.10	95.73	112.23
1	A	19	ILE	N-CA-C	10.85	131.90	109.34
1	A	252	ILE	CA-C-N	10.59	131.87	120.12
1	A	252	ILE	C-N-CA	10.59	131.87	120.12
1	A	43	THR	N-CA-C	-8.44	102.01	111.71
1	B	38	TYR	N-CA-C	-8.22	102.96	113.16
1	A	32	LYS	N-CA-C	-8.11	100.44	111.55
1	B	196	HIS	N-CA-C	-7.21	105.00	114.31
1	B	36	THR	N-CA-C	6.77	119.87	108.23
1	B	229	ALA	N-CA-C	-6.67	103.93	111.07
1	A	286	VAL	N-CA-C	-6.63	103.06	110.62
1	B	37	LYS	N-CA-C	-6.47	97.02	110.80
1	B	95	GLY	CA-C-N	6.45	126.16	119.64
1	B	95	GLY	C-N-CA	6.45	126.16	119.64
1	A	180	SER	N-CA-C	-6.37	105.57	113.15
1	A	151	LEU	N-CA-C	-6.24	100.18	109.86
1	B	29	LEU	N-CA-C	-6.06	104.58	111.07
1	B	180	SER	N-CA-C	-6.05	101.25	109.54
1	B	285	ALA	N-CA-C	-6.05	104.77	111.36
1	B	230	GLY	N-CA-C	-6.00	106.14	115.67
1	A	267	THR	N-CA-C	-5.90	106.42	113.97
1	B	139	CYS	N-CA-C	5.90	117.21	108.60
1	B	267	THR	N-CA-C	-5.88	106.27	113.50
1	A	198	VAL	N-CA-C	5.86	121.54	108.88
1	A	20	THR	N-CA-C	5.85	123.26	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ILE	N-CA-C	-5.77	99.87	108.46
1	B	276	GLN	N-CA-C	-5.74	105.10	111.36
1	A	235	GLY	N-CA-C	-5.73	105.85	112.50
1	A	243	THR	N-CA-C	-5.72	104.96	111.14
1	B	174	LEU	N-CA-C	5.65	118.17	109.07
1	B	107	SER	N-CA-C	-5.62	106.12	112.87
1	A	142	TYR	N-CA-C	-5.54	107.77	114.75
1	A	81	ASP	N-CA-C	5.46	118.23	110.10
1	A	237	ILE	N-CA-C	-5.33	105.41	110.42
1	B	154	GLY	N-CA-C	-5.33	101.48	112.34
1	B	193	TRP	N-CA-C	-5.31	98.07	109.81
1	B	27	GLU	N-CA-C	-5.17	106.92	113.18
1	A	84	TYR	N-CA-C	5.02	118.13	110.20
1	A	229	ALA	N-CA-C	-5.02	106.67	112.89

There are no chirality outliers.

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	2304	0	2291	324	0
1	B	2304	0	2291	306	0
2	A	12	0	0	2	0
2	B	11	0	0	5	0
All	All	4631	0	4582	624	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 68.

All (624) 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:10:PHE:HD2	1:A:13:GLU:HB2	1.09	1.13
1:B:46:THR:HG21	1:B:64:LEU:HB3	1.28	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:HG3	1:A:96:PRO:HA	1.30	1.10
1:A:46:THR:HG21	1:A:64:LEU:HB3	1.15	1.09
1:B:51:LYS:HG3	1:B:52:PRO:HD2	1.35	1.07
1:A:51:LYS:HG3	1:A:52:PRO:HD2	1.36	1.06
1:B:91:LYS:H	1:B:268:GLN:HE22	1.05	1.01
1:B:193:TRP:HE1	1:B:198:VAL:HG12	1.27	0.98
1:B:161:GLU:HB2	1:B:175:LYS:HD2	1.43	0.97
1:B:251:ILE:HG23	1:B:252:ILE:H	1.28	0.97
1:A:42:LYS:HB3	1:A:45:PRO:HG3	1.45	0.97
1:A:10:PHE:CD2	1:A:13:GLU:HB2	2.00	0.96
1:A:202:ILE:HA	1:A:205:ILE:HD13	1.46	0.96
1:A:236:VAL:HG13	1:A:282:VAL:HG22	1.47	0.96
1:A:87:ALA:HB2	1:A:102:THR:HG23	1.43	0.96
1:A:149:MET:HG3	1:A:150:GLN:HE21	1.32	0.95
1:A:100:ILE:HD11	1:A:222:PRO:HB2	1.47	0.94
1:B:51:LYS:HB2	1:B:51:LYS:NZ	1.81	0.94
1:A:194:PRO:HG2	1:A:199:PRO:HB3	1.50	0.93
1:B:51:LYS:HB2	1:B:51:LYS:HZ3	1.34	0.93
1:B:34:GLN:C	1:B:36:THR:H	1.73	0.93
1:A:134:MET:HA	1:B:150:GLN:NE2	1.87	0.90
1:B:42:LYS:HD2	1:B:45:PRO:HG3	1.52	0.89
1:A:192:ASN:O	1:A:193:TRP:HB2	1.72	0.89
1:B:87:ALA:HB2	1:B:102:THR:HG23	1.55	0.88
1:B:202:ILE:HA	1:B:205:ILE:HD13	1.54	0.88
1:B:91:LYS:HG2	1:B:96:PRO:HA	1.56	0.85
1:B:33:ARG:HB2	1:B:266:ARG:HH11	1.43	0.84
1:A:209:ILE:O	1:A:212:VAL:HG22	1.77	0.84
1:A:72:GLU:CG	1:A:83:SER:HB2	2.09	0.83
1:B:251:ILE:HG23	1:B:252:ILE:N	1.89	0.82
1:A:235:GLY:HA3	1:A:272:LEU:O	1.78	0.82
1:A:35:SER:O	1:A:40:ALA:HA	1.81	0.81
1:B:36:THR:OG1	1:B:40:ALA:HB2	1.81	0.80
1:B:133:GLU:HB2	1:B:138:LYS:HD3	1.63	0.80
1:B:134:MET:HG3	1:B:195:ASP:CG	2.07	0.80
1:A:252:ILE:CG2	1:A:254:GLU:HG2	2.10	0.79
1:A:51:LYS:CG	1:A:52:PRO:HD2	2.11	0.79
1:A:70:ARG:HH21	1:A:72:GLU:HG3	1.48	0.79
1:A:177:LYS:HG2	1:A:182:THR:HB	1.63	0.78
1:B:284:ASN:O	1:B:287:LEU:HB3	1.84	0.78
1:B:193:TRP:NE1	1:B:198:VAL:HG12	1.98	0.78
1:A:72:GLU:HG2	1:A:83:SER:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:HG21	1:B:70:ARG:HH12	1.49	0.78
1:A:31:LEU:HD22	1:A:266:ARG:HD3	1.65	0.77
1:A:46:THR:HG22	1:A:49:ALA:HB3	1.67	0.77
1:A:172:ARG:HG3	1:A:172:ARG:HH11	1.49	0.77
1:A:48:VAL:HG21	1:A:70:ARG:HH12	1.50	0.77
1:B:34:GLN:C	1:B:36:THR:N	2.42	0.76
1:B:149:MET:HB2	1:B:159:SER:HB3	1.67	0.76
1:A:148:GLU:OE1	1:A:148:GLU:HA	1.85	0.76
1:A:236:VAL:HG11	1:A:281:LEU:HD12	1.66	0.76
1:B:204:PRO:HG2	1:B:205:ILE:HD12	1.68	0.76
1:A:37:LYS:HE3	1:A:37:LYS:HA	1.67	0.76
1:B:11:LEU:O	1:B:15:GLN:HG3	1.84	0.76
1:B:133:GLU:O	1:B:134:MET:HE2	1.86	0.76
1:B:225:ILE:HG22	1:B:234:THR:HB	1.65	0.76
1:B:136:LYS:HD2	1:B:137:LYS:H	1.50	0.76
1:A:288:GLU:C	1:A:290:PHE:H	1.94	0.75
1:B:20:THR:O	1:B:24:PHE:HB2	1.87	0.75
1:B:32:LYS:HA	2:B:302:HOH:O	1.86	0.75
1:B:58:ASN:HD21	1:B:84:TYR:HE2	1.33	0.75
1:B:91:LYS:N	1:B:268:GLN:HE22	1.84	0.75
1:A:227:CYS:SG	1:A:234:THR:HG23	2.26	0.75
1:B:85:ILE:HD13	1:B:116:MET:SD	2.27	0.75
1:B:127:MET:HE2	1:B:189:HIS:NE2	2.02	0.74
1:B:235:GLY:HA3	1:B:272:LEU:O	1.85	0.74
1:A:284:ASN:O	1:A:287:LEU:HB3	1.86	0.74
1:A:13:GLU:HA	1:A:13:GLU:OE1	1.87	0.74
1:A:42:LYS:CB	1:A:45:PRO:HG3	2.15	0.74
1:B:105:PRO:HD2	1:B:139:CYS:SG	2.28	0.74
1:A:134:MET:HA	1:B:150:GLN:HE22	1.53	0.74
1:A:117:ILE:HD12	1:A:125:ILE:HD11	1.70	0.73
1:B:176:VAL:HG21	1:B:185:ILE:HD12	1.69	0.73
1:A:127:MET:HE2	1:A:189:HIS:NE2	2.03	0.73
1:B:158:VAL:HG13	1:B:176:VAL:HG13	1.70	0.73
1:B:133:GLU:HB2	1:B:138:LYS:CD	2.19	0.73
1:B:233:ARG:O	1:B:237:ILE:HG12	1.89	0.72
1:A:36:THR:HG22	1:A:37:LYS:N	2.03	0.72
1:B:101:ALA:HA	1:B:225:ILE:O	1.90	0.72
1:A:172:ARG:O	1:A:186:TYR:HA	1.90	0.71
1:A:105:PRO:HD2	1:A:139:CYS:SG	2.30	0.71
1:A:39:LYS:HG2	1:A:41:ASP:HB2	1.71	0.71
1:A:122:VAL:C	1:A:123:LEU:HD12	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:GLU:O	1:B:284:ASN:ND2	2.23	0.70
1:A:141:ARG:HA	1:A:143:TRP:CZ3	2.27	0.70
1:A:254:GLU:C	1:A:256:PHE:H	2.00	0.70
1:A:202:ILE:CA	1:A:205:ILE:HD13	2.22	0.70
1:B:34:GLN:O	1:B:36:THR:N	2.26	0.69
1:B:203:ASP:N	1:B:204:PRO:HD2	2.08	0.69
1:B:151:LEU:HB3	1:B:158:VAL:HG23	1.74	0.69
1:A:25:ALA:HA	1:A:276:GLN:NE2	2.08	0.69
1:A:265:MET:O	1:A:272:LEU:HD12	1.92	0.69
1:A:144:ALA:O	1:A:160:CYS:HB2	1.93	0.69
1:B:117:ILE:HD12	1:B:125:ILE:HD11	1.75	0.69
1:B:182:THR:HG22	1:B:183:ARG:H	1.57	0.69
1:B:91:LYS:H	1:B:268:GLN:NE2	1.88	0.68
1:B:209:ILE:O	1:B:212:VAL:HG22	1.94	0.68
1:A:194:PRO:HD2	1:A:199:PRO:HG3	1.76	0.67
1:A:71:VAL:HG22	1:A:89:PHE:CD1	2.30	0.67
1:A:65:PRO:HD3	1:A:86:ASN:ND2	2.10	0.67
1:A:118:TRP:CH2	1:A:183:ARG:HD3	2.29	0.67
1:A:102:THR:O	1:A:230:GLY:HA3	1.95	0.66
1:A:271:SER:HB3	1:A:274:GLN:HB3	1.77	0.66
1:A:118:TRP:O	1:A:183:ARG:NH2	2.26	0.66
1:B:125:ILE:HD13	1:B:224:CYS:HB3	1.76	0.66
1:B:194:PRO:CD	1:B:199:PRO:HD3	2.26	0.66
1:B:275:THR:HG22	1:B:277:GLU:N	2.10	0.66
1:A:177:LYS:HD3	1:A:182:THR:HG21	1.77	0.66
1:A:87:ALA:HB2	1:A:102:THR:CG2	2.24	0.66
1:B:271:SER:HB3	1:B:274:GLN:HB3	1.77	0.66
1:A:34:GLN:O	1:A:35:SER:C	2.39	0.66
1:B:127:MET:HE1	1:B:143:TRP:CH2	2.31	0.66
1:B:275:THR:HG22	1:B:277:GLU:H	1.60	0.65
1:A:43:THR:HB	1:A:44:TYR:CD1	2.31	0.65
1:A:202:ILE:HG22	1:A:205:ILE:HD13	1.78	0.65
1:B:182:THR:HG22	1:B:183:ARG:N	2.12	0.65
1:B:51:LYS:HG3	1:B:52:PRO:CD	2.20	0.65
1:B:90:ILE:HA	1:B:268:GLN:NE2	2.12	0.64
1:B:202:ILE:CA	1:B:205:ILE:HD13	2.28	0.64
1:B:43:THR:HB	1:B:44:TYR:CD1	2.33	0.64
1:A:197:ASP:O	1:A:277:GLU:HB3	1.97	0.64
1:A:176:VAL:HG21	1:A:185:ILE:HD12	1.80	0.64
1:A:254:GLU:C	1:A:256:PHE:N	2.55	0.64
1:B:263:ARG:HH11	1:B:263:ARG:HG3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:MET:HA	1:A:134:MET:HE2	1.80	0.63
1:A:59:ARG:HH12	1:A:139:CYS:HA	1.62	0.63
1:A:118:TRP:HA	1:A:183:ARG:NH2	2.13	0.63
1:B:33:ARG:HD3	1:B:33:ARG:O	1.98	0.63
1:B:236:VAL:HG13	1:B:282:VAL:HG22	1.81	0.63
1:A:134:MET:CA	1:B:150:GLN:NE2	2.62	0.63
1:A:276:GLN:O	1:A:280:GLU:HG3	1.99	0.62
1:B:246:LEU:HD13	1:B:252:ILE:CG1	2.29	0.62
1:A:9:LYS:HD2	1:A:253:PRO:HB3	1.81	0.62
1:A:123:LEU:CD1	1:A:221:VAL:HG21	2.30	0.62
1:A:72:GLU:CD	1:A:83:SER:HB2	2.24	0.62
1:B:241:ASP:HA	1:B:244:TRP:HB2	1.81	0.62
1:A:51:LYS:HB3	1:A:54:ASN:HD22	1.65	0.62
1:A:282:VAL:O	1:A:286:VAL:HG23	1.99	0.62
1:B:248:LYS:C	1:B:249:ASP:OD2	2.42	0.62
1:B:262:ILE:HD12	1:B:279:TYR:CD1	2.32	0.62
1:B:246:LEU:HD13	1:B:252:ILE:HG13	1.82	0.62
1:B:139:CYS:SG	1:B:140:GLU:N	2.73	0.62
1:A:15:GLN:C	1:A:17:LYS:H	2.08	0.61
1:B:194:PRO:HD2	1:B:199:PRO:HD3	1.82	0.61
1:A:205:ILE:HD12	1:A:205:ILE:H	1.65	0.61
1:A:246:LEU:HB3	1:A:251:ILE:HA	1.82	0.61
1:B:134:MET:N	2:B:295:HOH:O	2.33	0.61
1:A:114:TRP:CZ2	1:A:158:VAL:HG11	2.34	0.61
1:B:252:ILE:HD11	2:B:297:HOH:O	2.00	0.61
1:A:202:ILE:CG2	1:A:281:LEU:HD21	2.30	0.61
1:A:203:ASP:N	1:A:204:PRO:HD2	2.14	0.61
1:B:8:GLN:N	1:B:8:GLN:CD	2.59	0.61
1:A:172:ARG:HB2	1:A:187:GLN:HB3	1.83	0.60
1:B:33:ARG:NH2	1:B:270:PRO:HB2	2.16	0.60
1:B:144:ALA:O	1:B:160:CYS:HB2	2.01	0.60
1:A:177:LYS:HD3	1:A:182:THR:CG2	2.30	0.60
1:B:33:ARG:HB2	1:B:266:ARG:NH1	2.13	0.60
1:A:29:LEU:HD13	1:A:29:LEU:C	2.26	0.60
1:B:15:GLN:HG2	1:B:283:TYR:OH	2.02	0.60
1:B:37:LYS:NZ	1:B:39:LYS:O	2.35	0.60
1:B:252:ILE:HD13	1:B:256:PHE:HB3	1.83	0.60
1:B:59:ARG:HH12	1:B:139:CYS:HA	1.67	0.60
1:B:193:TRP:HE1	1:B:198:VAL:CG1	2.11	0.60
1:A:205:ILE:O	1:A:209:ILE:HG13	2.02	0.60
1:A:75:LEU:HD21	1:A:118:TRP:HD1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:O	1:A:17:LYS:N	2.36	0.59
1:A:269:ARG:HB3	1:A:272:LEU:HG	1.84	0.59
1:B:179:ASN:OD1	1:B:180:SER:N	2.35	0.59
1:A:252:ILE:HG23	1:A:254:GLU:HG2	1.82	0.59
1:B:46:THR:HG22	1:B:49:ALA:HB3	1.83	0.59
1:B:70:ARG:HG2	1:B:70:ARG:HH11	1.67	0.59
1:B:86:ASN:O	1:B:102:THR:HG23	2.03	0.59
1:A:106:LEU:HB2	1:A:109:THR:HG23	1.84	0.58
1:B:87:ALA:HB2	1:B:102:THR:CG2	2.30	0.58
1:A:201:SER:HA	2:A:300:HOH:O	2.03	0.58
1:B:260:SER:HA	1:B:263:ARG:HB2	1.85	0.58
1:A:123:LEU:HD11	1:A:221:VAL:HG21	1.85	0.58
1:A:127:MET:HG3	1:A:226:HIS:CE1	2.38	0.58
1:A:139:CYS:SG	1:A:140:GLU:N	2.75	0.58
1:A:237:ILE:O	1:A:238:CYS:C	2.45	0.58
1:A:118:TRP:CZ3	1:A:183:ARG:HB2	2.38	0.58
1:B:46:THR:CG2	1:B:49:ALA:HB3	2.34	0.58
1:A:18:LYS:HE2	1:A:27:GLU:HG3	1.85	0.58
1:B:76:ILE:HD13	1:B:76:ILE:H	1.69	0.58
1:B:100:ILE:HD11	1:B:222:PRO:HB2	1.85	0.58
1:B:190:TYR:CD1	1:B:208:LEU:HD22	2.39	0.58
1:A:205:ILE:HD12	1:A:205:ILE:N	2.19	0.58
1:B:151:LEU:HB3	1:B:153:PHE:HE1	1.68	0.58
1:B:197:ASP:OD2	1:B:197:ASP:N	2.33	0.58
1:B:236:VAL:CG2	1:B:278:GLN:HB3	2.34	0.57
1:A:86:ASN:O	1:A:102:THR:HG23	2.04	0.57
1:A:254:GLU:O	1:A:256:PHE:N	2.37	0.57
1:B:71:VAL:O	1:B:85:ILE:HG22	2.03	0.57
1:B:129:CYS:SG	1:B:227:CYS:HB2	2.45	0.57
1:A:149:MET:HG3	1:A:150:GLN:NE2	2.12	0.57
1:B:59:ARG:NH1	1:B:139:CYS:HA	2.20	0.57
1:B:202:ILE:HD12	1:B:202:ILE:C	2.29	0.57
1:A:124:ILE:HG22	1:A:124:ILE:O	2.04	0.57
1:A:135:GLY:HA2	1:B:150:GLN:O	2.05	0.57
1:B:124:ILE:HD12	1:B:188:PHE:HE1	1.70	0.56
1:A:15:GLN:C	1:A:17:LYS:N	2.62	0.56
1:A:20:THR:OG1	1:A:21:LYS:N	2.38	0.56
1:A:33:ARG:NH2	1:A:35:SER:HA	2.20	0.56
1:A:141:ARG:HB2	1:A:141:ARG:HH11	1.70	0.56
1:A:225:ILE:HG22	1:A:234:THR:HB	1.87	0.56
1:B:112:ASP:O	1:B:115:ARG:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ILE:HG21	1:B:244:TRP:HD1	1.70	0.56
1:A:275:THR:HG22	1:A:277:GLU:H	1.71	0.56
1:B:172:ARG:HG3	1:B:172:ARG:HH11	1.70	0.56
1:B:276:GLN:HG2	1:B:280:GLU:OE2	2.06	0.56
1:B:246:LEU:HD22	1:B:252:ILE:HG23	1.88	0.56
1:A:70:ARG:O	1:A:70:ARG:HG3	2.04	0.56
1:B:237:ILE:O	1:B:238:CYS:C	2.47	0.56
1:A:26:ASN:O	1:A:30:LYS:HG3	2.05	0.56
1:A:36:THR:HG22	1:A:37:LYS:H	1.70	0.56
1:A:41:ASP:O	1:A:42:LYS:C	2.48	0.56
1:B:82:SER:O	1:B:115:ARG:NH2	2.39	0.56
1:B:173:THR:HG22	1:B:186:TYR:HD2	1.72	0.55
1:A:236:VAL:CG1	1:A:281:LEU:HD12	2.33	0.55
1:B:271:SER:O	1:B:273:VAL:N	2.39	0.55
1:B:166:LYS:HB2	1:B:169:TYR:O	2.05	0.55
1:B:283:TYR:CD2	1:B:283:TYR:C	2.84	0.55
1:A:42:LYS:HB3	1:A:45:PRO:CG	2.26	0.55
1:A:50:GLU:HA	1:A:55:ILE:CD1	2.37	0.55
1:A:177:LYS:HA	1:A:182:THR:HA	1.87	0.55
1:B:190:TYR:CD2	1:B:193:TRP:HE3	2.25	0.55
1:A:70:ARG:HH11	1:A:70:ARG:HG2	1.71	0.55
1:A:100:ILE:CD1	1:A:222:PRO:HB2	2.29	0.55
1:B:41:ASP:O	1:B:42:LYS:HB2	2.06	0.55
1:A:46:THR:HG23	1:A:65:PRO:O	2.07	0.55
1:A:171:ILE:HD13	1:A:215:TYR:OH	2.06	0.55
1:B:251:ILE:CG2	1:B:252:ILE:H	2.04	0.55
1:A:172:ARG:HG3	1:A:172:ARG:NH1	2.21	0.55
1:B:198:VAL:HB	1:B:199:PRO:HD2	1.88	0.54
1:B:20:THR:OG1	1:B:21:LYS:N	2.38	0.54
1:A:215:TYR:N	1:A:215:TYR:HD2	2.05	0.54
1:B:102:THR:O	1:B:230:GLY:HA3	2.07	0.54
1:A:215:TYR:N	1:A:215:TYR:CD2	2.75	0.54
1:A:70:ARG:NH2	1:A:72:GLU:HG3	2.19	0.54
1:B:70:ARG:NH2	1:B:72:GLU:OE2	2.40	0.54
1:B:203:ASP:N	1:B:204:PRO:CD	2.71	0.54
1:A:125:ILE:CD1	1:A:224:CYS:HB3	2.38	0.54
1:A:151:LEU:HD23	1:A:153:PHE:CE1	2.43	0.54
1:B:12:ASP:HA	1:B:15:GLN:NE2	2.23	0.54
1:B:58:ASN:ND2	1:B:84:TYR:HE2	2.04	0.54
1:B:244:TRP:CE3	1:B:248:LYS:HE3	2.43	0.54
1:B:102:THR:HG22	1:B:103:GLN:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HD3	1:B:33:ARG:C	2.32	0.54
1:A:39:LYS:C	1:A:41:ASP:H	2.15	0.53
1:A:130:MET:O	1:A:131:GLU:C	2.51	0.53
1:B:190:TYR:CE2	1:B:193:TRP:CE3	2.96	0.53
1:A:21:LYS:HD2	1:A:276:GLN:OE1	2.09	0.53
1:A:240:ILE:HG13	1:A:282:VAL:HG13	1.89	0.53
1:A:74:SER:O	1:A:76:ILE:HG13	2.09	0.53
1:B:205:ILE:HD12	1:B:205:ILE:H	1.74	0.53
1:B:205:ILE:HD12	1:B:205:ILE:N	2.23	0.53
1:A:236:VAL:HG22	1:A:282:VAL:CG2	2.39	0.53
1:B:86:ASN:OD1	1:B:269:ARG:NH2	2.42	0.53
1:A:159:SER:O	1:A:175:LYS:N	2.42	0.53
1:A:198:VAL:O	1:A:198:VAL:HG22	2.07	0.53
1:B:46:THR:HG22	1:B:46:THR:O	2.08	0.53
1:A:14:ALA:HA	1:A:17:LYS:HE2	1.90	0.53
1:A:75:LEU:HD21	1:A:118:TRP:CD1	2.44	0.53
1:A:101:ALA:HA	1:A:225:ILE:O	2.09	0.53
1:B:15:GLN:HE22	1:B:287:LEU:HD12	1.73	0.53
1:A:222:PRO:C	1:A:223:ILE:HD12	2.34	0.53
1:B:17:LYS:HD2	1:B:17:LYS:N	2.24	0.53
1:B:18:LYS:O	1:B:19:ILE:O	2.27	0.53
1:A:211:ASP:O	1:A:214:CYS:HB2	2.08	0.53
1:A:251:ILE:HG23	1:A:251:ILE:O	2.09	0.53
1:B:149:MET:HB2	1:B:159:SER:CB	2.39	0.53
1:A:43:THR:HB	1:A:44:TYR:HD1	1.74	0.52
1:B:35:SER:O	1:B:40:ALA:HA	2.09	0.52
1:B:114:TRP:CZ2	1:B:158:VAL:HG11	2.44	0.52
1:A:242:TYR:C	1:A:242:TYR:CD2	2.87	0.52
1:A:258:VAL:O	1:A:262:ILE:HD13	2.10	0.52
1:B:46:THR:HB	1:B:50:GLU:OE2	2.10	0.52
1:B:250:GLY:O	1:B:251:ILE:O	2.27	0.52
1:A:9:LYS:HD3	1:A:9:LYS:N	2.24	0.52
1:A:134:MET:HE2	1:B:150:GLN:HE22	1.74	0.52
1:B:42:LYS:CD	1:B:45:PRO:HG3	2.33	0.52
1:B:188:PHE:CZ	1:B:212:VAL:HA	2.44	0.52
1:B:288:GLU:C	1:B:290:PHE:H	2.17	0.52
1:B:106:LEU:O	1:B:110:LEU:HG	2.10	0.52
1:B:106:LEU:C	1:B:108:THR:N	2.67	0.52
1:A:253:PRO:O	1:A:254:GLU:O	2.27	0.52
1:B:48:VAL:HA	1:B:51:LYS:HZ3	1.75	0.52
1:B:51:LYS:CG	1:B:52:PRO:HD2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:HB3	1:B:153:PHE:CE1	2.44	0.52
1:A:73:LEU:HD12	1:A:115:ARG:NH2	2.24	0.52
1:B:172:ARG:O	1:B:186:TYR:HA	2.10	0.52
1:A:90:ILE:HG12	1:A:272:LEU:HD11	1.91	0.52
1:A:146:PRO:HG2	1:A:163:GLU:CG	2.40	0.52
1:A:204:PRO:HG2	1:A:205:ILE:HD12	1.91	0.52
1:A:261:LEU:O	1:A:264:GLU:HG2	2.10	0.52
1:B:164:LYS:HB2	1:B:171:ILE:HB	1.91	0.51
1:A:192:ASN:O	1:A:193:TRP:CB	2.53	0.51
1:B:262:ILE:HD12	1:B:279:TYR:CE1	2.46	0.51
1:A:33:ARG:HH21	1:A:35:SER:HA	1.73	0.51
1:A:86:ASN:OD1	1:A:269:ARG:NH2	2.43	0.51
1:A:253:PRO:C	1:A:254:GLU:O	2.51	0.51
1:B:61:LYS:HG2	1:B:62:ASP:N	2.24	0.51
1:A:110:LEU:HB3	1:A:153:PHE:HD2	1.76	0.51
1:A:122:VAL:HG11	1:A:125:ILE:HD13	1.92	0.51
1:A:122:VAL:HG12	1:A:123:LEU:N	2.25	0.51
1:A:21:LYS:HG3	1:A:22:GLU:N	2.26	0.51
1:A:179:ASN:C	1:A:181:GLU:H	2.17	0.51
1:B:35:SER:OG	1:B:40:ALA:HB1	2.10	0.51
1:B:202:ILE:HG21	1:B:281:LEU:CD2	2.41	0.51
1:A:288:GLU:C	1:A:290:PHE:N	2.63	0.51
1:B:118:TRP:O	1:B:183:ARG:NH2	2.43	0.51
1:A:46:THR:CG2	1:A:49:ALA:HB3	2.38	0.51
1:B:13:GLU:OE1	1:B:13:GLU:N	2.44	0.51
1:A:59:ARG:NH1	1:A:139:CYS:HA	2.26	0.50
1:B:21:LYS:HG3	1:B:276:GLN:HE22	1.75	0.50
1:B:106:LEU:C	1:B:108:THR:H	2.19	0.50
1:B:244:TRP:CE3	1:B:244:TRP:HA	2.46	0.50
1:B:259:PHE:O	1:B:263:ARG:N	2.42	0.50
1:A:8:GLN:NE2	1:A:8:GLN:HA	2.26	0.50
1:A:17:LYS:N	1:A:17:LYS:HD3	2.26	0.50
1:A:202:ILE:HG21	1:A:281:LEU:HD21	1.94	0.50
1:A:262:ILE:HG22	1:A:266:ARG:HD2	1.93	0.50
1:B:252:ILE:O	1:B:253:PRO:C	2.54	0.50
1:A:117:ILE:HG21	1:A:185:ILE:HD13	1.94	0.50
1:B:37:LYS:NZ	1:B:37:LYS:HB2	2.27	0.50
1:A:127:MET:HE1	1:A:143:TRP:CH2	2.45	0.50
1:B:262:ILE:HD12	1:B:279:TYR:HD1	1.77	0.50
1:A:27:GLU:OE1	1:A:27:GLU:HA	2.11	0.50
1:A:142:TYR:HA	1:A:153:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ILE:HB	1:B:99:TYR:HB2	1.94	0.50
1:B:136:LYS:HD2	1:B:137:LYS:N	2.23	0.50
1:A:278:GLN:O	1:A:282:VAL:HG23	2.12	0.50
1:B:134:MET:HG3	1:B:195:ASP:OD1	2.12	0.50
1:B:278:GLN:O	1:B:282:VAL:HG23	2.11	0.50
1:B:130:MET:HG2	1:B:191:LYS:HG2	1.94	0.50
1:B:188:PHE:CD2	1:B:212:VAL:HG12	2.47	0.50
1:A:223:ILE:HG22	1:A:225:ILE:HG13	1.93	0.49
1:B:86:ASN:O	1:B:102:THR:CG2	2.60	0.49
1:B:106:LEU:N	1:B:109:THR:OG1	2.34	0.49
1:B:125:ILE:CD1	1:B:224:CYS:HB3	2.41	0.49
1:A:7:LEU:O	1:A:9:LYS:NZ	2.45	0.49
1:A:37:LYS:HA	1:A:37:LYS:CE	2.41	0.49
1:A:262:ILE:O	1:A:266:ARG:HD2	2.12	0.49
1:B:33:ARG:O	1:B:34:GLN:C	2.55	0.49
1:B:100:ILE:CD1	1:B:222:PRO:HB2	2.42	0.49
1:A:121:SER:HA	1:A:183:ARG:NH2	2.27	0.49
1:B:89:PHE:CE2	1:B:100:ILE:HG12	2.47	0.49
1:A:118:TRP:HZ3	1:A:183:ARG:HB2	1.77	0.49
1:B:29:LEU:C	1:B:29:LEU:HD13	2.37	0.49
1:B:51:LYS:CG	1:B:54:ASN:HD22	2.26	0.49
1:B:202:ILE:HG21	1:B:281:LEU:HD21	1.94	0.49
1:A:18:LYS:HD3	1:A:23:GLU:OE2	2.13	0.49
1:B:133:GLU:HB2	1:B:138:LYS:CG	2.42	0.49
1:A:172:ARG:HH11	1:A:172:ARG:CG	2.22	0.49
1:A:202:ILE:HG22	1:A:205:ILE:CD1	2.42	0.49
1:B:7:LEU:O	1:B:7:LEU:HG	2.13	0.49
1:A:141:ARG:HH11	1:A:141:ARG:CB	2.25	0.49
1:B:77:THR:O	1:B:78:SER:HB3	2.11	0.49
1:A:289:LEU:O	1:A:290:PHE:C	2.55	0.49
1:B:7:LEU:HD11	2:B:298:HOH:O	2.12	0.49
1:A:105:PRO:HG3	1:A:142:TYR:CD1	2.47	0.49
1:B:18:LYS:HA	1:B:23:GLU:HG2	1.95	0.49
1:B:196:HIS:ND1	1:B:196:HIS:C	2.71	0.49
1:A:21:LYS:O	1:A:25:ALA:N	2.33	0.49
1:B:133:GLU:HA	1:B:133:GLU:OE1	2.13	0.49
1:B:106:LEU:HD12	1:B:109:THR:HG23	1.95	0.48
1:B:228:SER:OG	1:B:229:ALA:N	2.47	0.48
1:A:15:GLN:C	1:A:15:GLN:CD	2.82	0.48
1:A:123:LEU:HD12	1:A:123:LEU:N	2.26	0.48
1:A:190:TYR:CE2	1:A:193:TRP:CE3	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:THR:HG22	1:A:277:GLU:N	2.28	0.48
1:B:33:ARG:CZ	1:B:270:PRO:HB2	2.43	0.48
1:A:65:PRO:HD3	1:A:86:ASN:HD21	1.77	0.48
1:B:42:LYS:HE3	1:B:45:PRO:HB3	1.94	0.48
1:A:124:ILE:HG13	1:A:188:PHE:CE1	2.48	0.48
1:A:277:GLU:N	1:A:277:GLU:OE1	2.46	0.48
1:B:251:ILE:CG2	1:B:252:ILE:N	2.62	0.48
1:A:29:LEU:HD13	1:A:29:LEU:O	2.12	0.48
1:A:100:ILE:HD11	1:A:222:PRO:CB	2.33	0.48
1:B:266:ARG:HA	1:B:269:ARG:O	2.14	0.48
1:A:21:LYS:O	1:A:24:PHE:N	2.47	0.48
1:A:7:LEU:C	1:A:9:LYS:NZ	2.72	0.48
1:A:48:VAL:HG21	1:A:70:ARG:NH1	2.24	0.48
1:B:10:PHE:HB3	1:B:13:GLU:HB2	1.95	0.48
1:B:21:LYS:HG3	1:B:25:ALA:HB2	1.96	0.47
1:B:192:ASN:O	1:B:193:TRP:HB2	2.14	0.47
1:A:21:LYS:O	1:A:22:GLU:C	2.58	0.47
1:A:86:ASN:O	1:A:102:THR:CG2	2.62	0.47
1:A:212:VAL:HG23	1:A:213:ARG:N	2.28	0.47
1:B:133:GLU:C	1:B:134:MET:HE2	2.39	0.47
1:A:130:MET:HE2	1:A:191:LYS:O	2.14	0.47
1:A:134:MET:CA	1:B:150:GLN:HE21	2.26	0.47
1:A:141:ARG:HB2	1:A:141:ARG:NH1	2.30	0.47
1:B:179:ASN:CG	1:B:180:SER:H	2.22	0.47
1:B:243:THR:O	1:B:244:TRP:C	2.57	0.47
1:B:33:ARG:C	1:B:33:ARG:CD	2.87	0.47
1:B:70:ARG:HG2	1:B:70:ARG:NH1	2.28	0.47
1:B:115:ARG:HG3	1:B:115:ARG:HH11	1.80	0.47
1:A:10:PHE:HD2	1:A:13:GLU:CB	2.02	0.47
1:A:44:TYR:OH	1:A:267:THR:HG23	2.15	0.47
1:A:112:ASP:HA	1:A:115:ARG:NH1	2.30	0.47
1:A:143:TRP:CD1	1:A:172:ARG:NH1	2.82	0.47
1:A:151:LEU:HD23	1:A:153:PHE:CZ	2.49	0.47
1:A:203:ASP:N	1:A:204:PRO:CD	2.76	0.47
1:B:35:SER:C	1:B:40:ALA:HA	2.40	0.47
1:B:273:VAL:O	1:B:275:THR:N	2.48	0.47
1:A:114:TRP:O	1:A:115:ARG:C	2.57	0.47
1:A:177:LYS:HG2	1:A:182:THR:CB	2.40	0.47
1:B:10:PHE:HA	1:B:13:GLU:CD	2.40	0.47
1:B:179:ASN:OD1	1:B:181:GLU:HB3	2.15	0.47
1:B:249:ASP:OD2	1:B:249:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:CD	1:A:9:LYS:H	2.28	0.47
1:A:20:THR:O	1:A:24:PHE:HB2	2.15	0.47
1:A:212:VAL:CG2	1:A:213:ARG:N	2.78	0.47
1:B:241:ASP:O	1:B:244:TRP:N	2.47	0.47
1:A:254:GLU:OE2	1:A:254:GLU:HA	2.15	0.47
1:A:287:LEU:O	1:A:290:PHE:N	2.48	0.47
1:A:171:ILE:HD11	1:A:211:ASP:OD1	2.15	0.47
1:B:172:ARG:HB2	1:B:187:GLN:HB3	1.96	0.47
1:A:241:ASP:HA	1:A:244:TRP:HB2	1.97	0.46
1:A:258:VAL:O	1:A:261:LEU:HB3	2.15	0.46
1:A:117:ILE:HD12	1:A:125:ILE:CD1	2.44	0.46
1:A:190:TYR:HE2	1:A:193:TRP:CE3	2.33	0.46
1:A:288:GLU:O	1:A:290:PHE:N	2.48	0.46
1:B:10:PHE:HA	1:B:13:GLU:OE1	2.15	0.46
1:B:51:LYS:HD2	1:B:54:ASN:ND2	2.29	0.46
1:B:161:GLU:CB	1:B:175:LYS:HD2	2.30	0.46
1:A:32:LYS:C	1:A:34:GLN:H	2.24	0.46
1:A:70:ARG:HG2	1:A:70:ARG:NH1	2.30	0.46
1:A:71:VAL:HG13	1:A:89:PHE:CE1	2.51	0.46
1:A:252:ILE:O	1:A:252:ILE:HG22	2.14	0.46
1:B:19:ILE:HD13	1:B:19:ILE:H	1.80	0.46
1:B:127:MET:HG3	1:B:226:HIS:CE1	2.51	0.46
1:B:202:ILE:CG2	1:B:281:LEU:HD21	2.46	0.46
1:A:195:ASP:HA	1:A:233:ARG:HH21	1.80	0.46
1:A:264:GLU:O	1:A:267:THR:HB	2.16	0.46
1:B:48:VAL:HA	1:B:51:LYS:NZ	2.31	0.46
1:A:59:ARG:N	1:A:103:GLN:HE22	2.12	0.46
1:B:188:PHE:CG	1:B:212:VAL:HG12	2.51	0.46
1:B:263:ARG:HG3	1:B:263:ARG:NH1	2.29	0.46
1:A:15:GLN:HG2	1:A:283:TYR:OH	2.16	0.46
1:A:124:ILE:HG13	1:A:188:PHE:HE1	1.81	0.46
1:B:54:ASN:HA	1:B:57:LYS:HD2	1.98	0.46
1:A:123:LEU:CD1	1:A:123:LEU:N	2.79	0.46
1:B:51:LYS:HZ3	1:B:51:LYS:CB	2.15	0.46
1:B:275:THR:CG2	1:B:277:GLU:HB2	2.45	0.46
1:A:233:ARG:O	1:A:237:ILE:HG12	2.16	0.46
1:A:89:PHE:CE2	1:A:100:ILE:HG12	2.50	0.45
1:A:153:PHE:CD1	1:A:153:PHE:N	2.84	0.45
1:A:202:ILE:HA	1:A:205:ILE:CD1	2.31	0.45
1:B:130:MET:O	1:B:131:GLU:C	2.59	0.45
1:A:39:LYS:HG2	1:A:41:ASP:CB	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:SER:HB2	1:B:43:THR:OG1	2.16	0.45
1:B:202:ILE:HA	1:B:205:ILE:CD1	2.37	0.45
1:B:84:TYR:OH	1:B:86:ASN:ND2	2.50	0.45
1:A:105:PRO:O	1:A:106:LEU:HD23	2.17	0.45
1:B:215:TYR:N	1:B:215:TYR:CD2	2.83	0.45
1:A:133:GLU:HB2	1:A:138:LYS:HG3	1.98	0.45
1:A:243:THR:O	1:A:244:TRP:C	2.59	0.45
1:B:128:ALA:HA	1:B:190:TYR:HB3	1.98	0.45
1:A:87:ALA:HA	1:A:101:ALA:O	2.16	0.45
1:A:177:LYS:HB3	1:A:182:THR:HG22	1.99	0.45
1:B:12:ASP:HA	1:B:15:GLN:HE21	1.82	0.45
1:A:110:LEU:HD22	1:A:153:PHE:CE2	2.52	0.45
1:A:115:ARG:HG2	1:A:156:PHE:HE1	1.81	0.45
1:A:116:MET:O	1:A:117:ILE:C	2.59	0.45
1:A:281:LEU:HD13	1:A:281:LEU:C	2.42	0.45
1:B:14:ALA:HA	1:B:17:LYS:HD3	1.99	0.45
1:B:70:ARG:HE	1:B:72:GLU:HG2	1.81	0.45
1:B:190:TYR:CE2	1:B:193:TRP:HE3	2.33	0.45
1:B:276:GLN:O	1:B:280:GLU:HG3	2.16	0.45
1:A:252:ILE:HD13	1:A:252:ILE:HA	1.80	0.45
1:A:157:SER:O	1:A:176:VAL:HA	2.17	0.45
1:A:202:ILE:HG23	1:A:281:LEU:HD21	1.98	0.45
1:A:79:ASP:O	1:A:81:ASP:N	2.50	0.45
1:A:137:LYS:HE2	1:A:139:CYS:O	2.17	0.45
1:A:147:GLY:O	1:A:148:GLU:O	2.35	0.45
1:B:41:ASP:O	1:B:42:LYS:CB	2.65	0.45
1:A:72:GLU:HG2	1:A:73:LEU:H	1.82	0.44
1:A:172:ARG:HD2	1:A:174:LEU:HD21	1.98	0.44
1:B:222:PRO:C	1:B:223:ILE:HD12	2.42	0.44
1:B:271:SER:O	1:B:274:GLN:N	2.51	0.44
1:A:39:LYS:C	1:A:41:ASP:N	2.76	0.44
1:B:141:ARG:HE	1:B:141:ARG:HB3	1.61	0.44
1:B:150:GLN:O	1:B:150:GLN:HG3	2.17	0.44
1:A:7:LEU:C	1:A:9:LYS:HZ2	2.25	0.44
1:B:15:GLN:NE2	1:B:287:LEU:HD12	2.32	0.44
1:B:190:TYR:HE2	1:B:193:TRP:CE3	2.35	0.44
1:A:125:ILE:HD12	1:A:224:CYS:HB3	1.99	0.44
1:A:179:ASN:C	1:A:181:GLU:N	2.76	0.44
1:B:43:THR:HB	1:B:44:TYR:HD1	1.82	0.44
1:B:182:THR:CG2	1:B:183:ARG:H	2.29	0.44
1:A:172:ARG:NH1	1:A:172:ARG:CG	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PHE:O	1:A:260:SER:C	2.61	0.44
1:B:9:LYS:NZ	1:B:251:ILE:CG2	2.81	0.44
1:B:123:LEU:CD2	1:B:186:TYR:HE1	2.30	0.44
1:B:171:ILE:HD11	1:B:211:ASP:OD1	2.18	0.44
1:A:202:ILE:CG2	1:A:205:ILE:HD13	2.46	0.44
1:A:22:GLU:HA	1:A:25:ALA:HB3	1.99	0.43
1:A:48:VAL:HG22	1:A:51:LYS:NZ	2.33	0.43
1:A:120:TYR:O	1:A:121:SER:C	2.61	0.43
1:A:253:PRO:O	1:A:254:GLU:C	2.61	0.43
1:B:74:SER:H	1:B:119:GLU:CD	2.26	0.43
1:B:100:ILE:HD11	1:B:222:PRO:CB	2.47	0.43
1:B:261:LEU:O	1:B:265:MET:HG3	2.17	0.43
1:A:122:VAL:CG1	1:A:123:LEU:N	2.81	0.43
1:A:263:ARG:HD3	1:A:263:ARG:C	2.43	0.43
1:B:39:LYS:HB2	2:B:304:HOH:O	2.17	0.43
1:B:141:ARG:HA	1:B:143:TRP:CZ3	2.53	0.43
1:B:227:CYS:SG	1:B:234:THR:HG23	2.58	0.43
1:B:247:LEU:C	1:B:249:ASP:H	2.26	0.43
1:B:252:ILE:CD1	1:B:256:PHE:HB3	2.48	0.43
1:A:73:LEU:CD1	1:A:115:ARG:NH2	2.81	0.43
1:B:19:ILE:HB	1:B:20:THR:H	1.66	0.43
1:B:76:ILE:C	1:B:78:SER:H	2.27	0.43
1:B:287:LEU:O	1:B:290:PHE:N	2.49	0.43
1:A:29:LEU:O	1:A:32:LYS:HG2	2.18	0.43
1:B:75:LEU:HD12	1:B:115:ARG:O	2.19	0.43
1:B:260:SER:HA	1:B:263:ARG:CB	2.47	0.43
1:A:18:LYS:HE2	1:A:27:GLU:CG	2.48	0.43
1:A:105:PRO:C	1:A:106:LEU:HD23	2.44	0.43
1:B:9:LYS:C	1:B:11:LEU:H	2.27	0.43
1:B:89:PHE:HE2	1:B:100:ILE:HG12	1.82	0.43
1:A:22:GLU:CD	1:A:23:GLU:N	2.77	0.43
1:A:125:ILE:HD13	1:A:224:CYS:HB3	1.99	0.43
1:B:42:LYS:HD2	1:B:45:PRO:CG	2.36	0.43
1:A:277:GLU:N	1:A:277:GLU:CD	2.77	0.43
1:A:290:PHE:O	1:A:290:PHE:CD1	2.72	0.43
1:B:106:LEU:HD12	1:B:109:THR:CG2	2.49	0.43
1:A:74:SER:HB2	1:A:119:GLU:OE1	2.19	0.43
1:A:110:LEU:HD22	1:A:153:PHE:HE2	1.84	0.43
1:A:242:TYR:C	1:A:242:TYR:HD2	2.26	0.43
1:A:254:GLU:OE2	1:A:254:GLU:CA	2.67	0.43
1:A:252:ILE:HG22	1:A:254:GLU:HG2	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ARG:HH11	1:B:172:ARG:CG	2.28	0.42
1:A:20:THR:HG23	1:A:21:LYS:N	2.34	0.42
1:A:186:TYR:CD1	1:A:186:TYR:N	2.87	0.42
1:B:122:VAL:HG12	1:B:123:LEU:N	2.34	0.42
1:A:59:ARG:H	1:A:103:GLN:NE2	2.18	0.42
1:A:89:PHE:HE2	1:A:100:ILE:HG12	1.84	0.42
1:A:227:CYS:SG	1:A:234:THR:CG2	3.05	0.42
1:A:290:PHE:O	1:A:290:PHE:HD1	2.03	0.42
1:A:194:PRO:O	1:A:195:ASP:CG	2.62	0.42
1:B:209:ILE:HD12	1:B:240:ILE:CG2	2.50	0.42
1:A:276:GLN:HE21	1:A:276:GLN:HB2	1.68	0.42
1:A:25:ALA:O	1:A:29:LEU:N	2.52	0.42
1:A:263:ARG:HD3	1:A:263:ARG:O	2.20	0.42
1:B:51:LYS:HG2	1:B:54:ASN:HD22	1.84	0.42
1:B:202:ILE:C	1:B:204:PRO:HD2	2.45	0.42
1:B:241:ASP:O	1:B:242:TYR:C	2.63	0.42
1:B:247:LEU:O	1:B:249:ASP:N	2.52	0.42
1:A:248:LYS:C	1:A:249:ASP:OD2	2.63	0.42
1:A:236:VAL:CG1	1:A:282:VAL:HG22	2.34	0.42
1:B:141:ARG:NH2	1:B:145:GLU:OE2	2.52	0.42
1:B:242:TYR:O	1:B:245:MET:HB2	2.20	0.42
1:B:247:LEU:C	1:B:249:ASP:N	2.77	0.42
1:A:59:ARG:H	1:A:103:GLN:HE22	1.67	0.42
1:A:233:ARG:HG3	2:A:297:HOH:O	2.20	0.42
1:A:271:SER:C	1:A:273:VAL:N	2.78	0.42
1:A:39:LYS:O	1:A:41:ASP:N	2.48	0.41
1:A:231:CYS:O	1:A:272:LEU:O	2.38	0.41
1:A:263:ARG:HG3	1:A:263:ARG:HH11	1.85	0.41
1:B:8:GLN:NE2	1:B:8:GLN:HA	2.35	0.41
1:B:75:LEU:HD11	1:B:118:TRP:HD1	1.84	0.41
1:B:164:LYS:O	1:B:170:ILE:HA	2.19	0.41
1:A:154:GLY:C	1:A:156:PHE:N	2.77	0.41
1:B:11:LEU:HG	1:B:15:GLN:OE1	2.19	0.41
1:B:65:PRO:HD3	1:B:86:ASN:HD21	1.85	0.41
1:B:130:MET:C	1:B:132:TYR:N	2.78	0.41
1:B:197:ASP:HB2	1:B:198:VAL:H	1.75	0.41
1:B:275:THR:HG21	1:B:277:GLU:HB2	2.02	0.41
1:B:58:ASN:ND2	1:B:86:ASN:HD22	2.18	0.41
1:B:175:LYS:HE2	1:B:175:LYS:HB2	1.89	0.41
1:B:213:ARG:HD3	1:B:213:ARG:HA	1.88	0.41
1:B:51:LYS:HB2	1:B:51:LYS:HZ2	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:VAL:O	1:B:261:LEU:HB3	2.21	0.41
1:B:48:VAL:O	1:B:48:VAL:HG12	2.20	0.41
1:B:253:PRO:O	1:B:254:GLU:O	2.38	0.41
1:A:59:ARG:H	1:A:103:GLN:CD	2.27	0.41
1:A:118:TRP:HZ2	1:A:181:GLU:CD	2.28	0.41
1:A:149:MET:HG3	1:A:150:GLN:H	1.84	0.41
1:A:251:ILE:O	1:A:251:ILE:HG12	2.21	0.41
1:B:262:ILE:O	1:B:266:ARG:HG2	2.20	0.41
1:A:44:TYR:CD1	1:A:44:TYR:N	2.89	0.41
1:A:51:LYS:CG	1:A:52:PRO:CD	2.91	0.41
1:A:71:VAL:O	1:A:85:ILE:HG22	2.21	0.41
1:A:265:MET:C	1:A:272:LEU:HD12	2.45	0.41
1:A:68:TYR:CD1	1:A:68:TYR:C	2.98	0.41
1:A:131:GLU:CD	1:A:141:ARG:HH12	2.29	0.41
1:B:117:ILE:CD1	1:B:125:ILE:HD11	2.47	0.41
1:B:225:ILE:CG2	1:B:234:THR:HB	2.43	0.41
1:B:290:PHE:N	1:B:290:PHE:CD2	2.87	0.41
1:A:31:LEU:HD22	1:A:266:ARG:CD	2.44	0.41
1:A:36:THR:O	1:A:37:LYS:HB2	2.21	0.41
1:A:79:ASP:CG	1:A:80:GLU:H	2.26	0.41
1:A:122:VAL:HG11	1:A:125:ILE:CD1	2.49	0.41
1:A:124:ILE:O	1:A:124:ILE:CG2	2.64	0.41
1:A:127:MET:HE2	1:A:189:HIS:CE1	2.55	0.41
1:A:226:HIS:HA	1:A:234:THR:HG21	2.02	0.41
1:A:251:ILE:O	1:A:252:ILE:C	2.64	0.41
1:B:9:LYS:HD3	1:B:9:LYS:N	2.36	0.41
1:B:48:VAL:HG21	1:B:70:ARG:NH1	2.27	0.41
1:A:223:ILE:HD12	1:A:223:ILE:N	2.35	0.41
1:B:90:ILE:HD12	1:B:90:ILE:N	2.35	0.41
1:B:102:THR:O	1:B:230:GLY:CA	2.68	0.41
1:B:110:LEU:HD21	1:B:140:GLU:HG3	2.02	0.41
1:B:231:CYS:O	1:B:232:GLY:C	2.64	0.40
1:B:246:LEU:HD13	1:B:252:ILE:HG12	2.03	0.40
1:A:163:GLU:CD	1:A:163:GLU:O	2.64	0.40
1:B:44:TYR:OH	1:B:267:THR:HG23	2.21	0.40
1:B:144:ALA:HA	1:B:151:LEU:HD22	2.03	0.40
1:B:243:THR:C	1:B:245:MET:N	2.78	0.40
1:A:106:LEU:O	1:A:110:LEU:HG	2.21	0.40
1:A:148:GLU:HB3	1:A:149:MET:H	1.60	0.40
1:B:74:SER:O	1:B:76:ILE:HG23	2.21	0.40
1:A:230:GLY:O	1:A:231:CYS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.86	0.40
1:B:34:GLN:N	1:B:34:GLN:OE1	2.54	0.40
1:B:60:TYR:HB2	1:B:63:ILE:HG12	2.03	0.40
1:B:212:VAL:HG23	1:B:213:ARG:N	2.37	0.40
1:A:246:LEU:HB3	1:A:251:ILE:HG13	2.03	0.40
1:B:146:PRO:HG3	1:B:160:CYS:SG	2.62	0.40
1:B:157:SER:O	1:B:176:VAL:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	276/313 (88%)	191 (69%)	59 (21%)	26 (9%)	0	2
1	B	276/313 (88%)	205 (74%)	50 (18%)	21 (8%)	1	4
All	All	552/626 (88%)	396 (72%)	109 (20%)	47 (8%)	0	3

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	42	LYS
1	A	80	GLU
1	A	148	GLU
1	A	193	TRP
1	A	200	SER
1	B	19	ILE
1	B	42	LYS
1	B	193	TRP
1	B	194	PRO
1	B	251	ILE

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Mol	Chain	Res	Type
1	B	254	GLU
1	B	272	LEU
1	B	274	GLN
1	A	16	SER
1	A	18	LYS
1	A	167	SER
1	A	179	ASN
1	A	231	CYS
1	A	248	LYS
1	A	254	GLU
1	A	289	LEU
1	B	35	SER
1	B	133	GLU
1	B	179	ASN
1	B	195	ASP
1	B	232	GLY
1	B	248	LYS
1	B	253	PRO
1	A	52	PRO
1	A	59	ARG
1	B	52	PRO
1	B	54	ASN
1	B	238	CYS
1	B	259	PHE
1	B	287	LEU
1	A	247	LEU
1	A	255	ASN
1	A	35	SER
1	A	131	GLU
1	A	194	PRO
1	B	37	LYS
1	A	195	ASP
1	A	202	ILE
1	A	273	VAL
1	A	222	PRO
1	A	252	ILE

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	256/287 (89%)	218 (85%)	38 (15%)	3	15
1	B	256/287 (89%)	219 (86%)	37 (14%)	3	15
All	All	512/574 (89%)	437 (85%)	75 (15%)	3	15

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	9	LYS
1	A	10	PHE
1	A	13	GLU
1	A	18	LYS
1	A	22	GLU
1	A	37	LYS
1	A	55	ILE
1	A	68	TYR
1	A	70	ARG
1	A	75	LEU
1	A	100	ILE
1	A	123	LEU
1	A	124	ILE
1	A	141	ARG
1	A	148	GLU
1	A	150	GLN
1	A	158	VAL
1	A	163	GLU
1	A	166	LYS
1	A	173	THR
1	A	176	VAL
1	A	181	GLU
1	A	183	ARG
1	A	194	PRO
1	A	202	ILE
1	A	206	LEU
1	A	211	ASP
1	A	213	ARG
1	A	215	TYR
1	A	221	VAL
1	A	244	TRP
1	A	252	ILE

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Mol	Chain	Res	Type
1	A	255	ASN
1	A	256	PHE
1	A	263	ARG
1	A	265	MET
1	A	268	GLN
1	B	8	GLN
1	B	17	LYS
1	B	19	ILE
1	B	22	GLU
1	B	29	LEU
1	B	34	GLN
1	B	37	LYS
1	B	42	LYS
1	B	43	THR
1	B	51	LYS
1	B	52	PRO
1	B	55	ILE
1	B	61	LYS
1	B	68	TYR
1	B	70	ARG
1	B	76	ILE
1	B	133	GLU
1	B	148	GLU
1	B	149	MET
1	B	151	LEU
1	B	158	VAL
1	B	161	GLU
1	B	163	GLU
1	B	176	VAL
1	B	183	ARG
1	B	186	TYR
1	B	196	HIS
1	B	197	ASP
1	B	206	LEU
1	B	215	TYR
1	B	234	THR
1	B	244	TRP
1	B	249	ASP
1	B	252	ILE
1	B	253	PRO
1	B	263	ARG
1	B	265	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	150	GLN
1	A	255	ASN
1	A	276	GLN
1	A	278	GLN
1	A	284	ASN
1	B	8	GLN
1	B	15	GLN
1	B	54	ASN
1	B	58	ASN
1	B	150	GLN
1	B	187	GLN
1	B	268	GLN
1	B	276	GLN
1	B	278	GLN
1	B	284	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	280/313 (89%)	0.44	9 (3%)	50	29	9, 52, 93, 104	0
1	B	280/313 (89%)	0.44	18 (6%)	25	13	5, 52, 95, 104	0
All	All	560/626 (89%)	0.44	27 (4%)	35	19	5, 52, 95, 104	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	ILE	4.4
1	A	146	PRO	3.4
1	B	41	ASP	3.4
1	B	198	VAL	3.3
1	B	146	PRO	3.0
1	B	23	GLU	2.9
1	B	15	GLN	2.8
1	A	197	ASP	2.8
1	B	195	ASP	2.7
1	A	254	GLU	2.5
1	B	17	LYS	2.4
1	B	61	LYS	2.4
1	B	255	ASN	2.3
1	A	255	ASN	2.3
1	A	250	GLY	2.3
1	B	178	PHE	2.3
1	B	139	CYS	2.2
1	B	180	SER	2.2
1	B	19	ILE	2.2
1	B	95	GLY	2.1
1	B	197	ASP	2.1
1	A	38	TYR	2.1
1	B	254	GLU	2.1
1	A	199	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	106	LEU	2.0
1	B	9	LYS	2.0
1	A	253	PRO	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.