



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:10 PM UTC

PDB ID : 2PK2 / pdb_00002pk2
Title : Cyclin box structure of the P-TEFb subunit Cyclin T1 derived from a fusion complex with EIAV Tat
Authors : Anand, K.; Schulte, A.; Fujinaga, K.; Scheffzek, K.; Geyer, M.
Deposited on : 2007-04-17
Resolution : 2.67 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

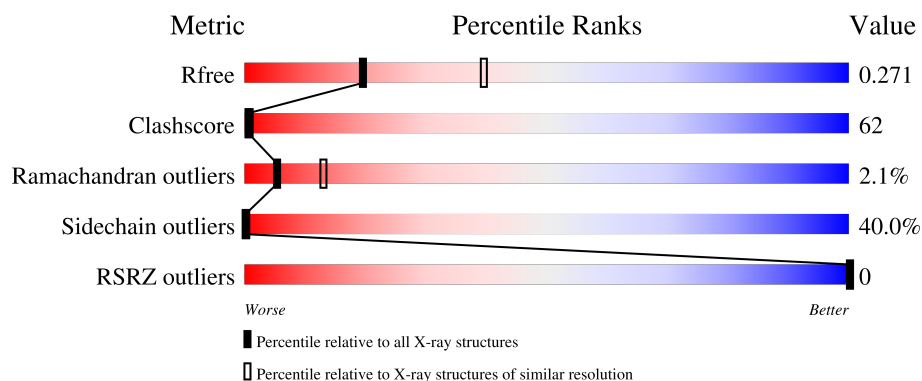
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	358	
1	B	358	
1	C	358	
1	D	358	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8396 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 Cyclin-T1, Protein Tat.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2076	1331	360	375	10			
1	B	256	Total	C	N	O	S	0	0	0
			2080	1333	360	377	10			
1	C	256	Total	C	N	O	S	0	0	0
			2082	1334	361	377	10			
1	D	256	Total	C	N	O	S	0	0	0
			2079	1332	360	377	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ARG	GLN	SEE REMARK 999	UNP O60563
A	282	GLY	-	linker	UNP O60563
A	283	GLY	-	linker	UNP O60563
A	284	THR	-	linker	UNP O60563
A	285	GLY	-	linker	UNP O60563
A	286	GLY	-	linker	UNP O60563
A	287	GLY	-	linker	UNP O60563
A	288	SER	-	linker	UNP O60563
A	289	GLY	-	linker	UNP O60563
A	290	GLY	-	linker	UNP O60563
A	291	GLY	-	linker	UNP O60563
A	292	SER	-	linker	UNP O60563
A	293	GLY	-	linker	UNP O60563
A	294	GLY	-	linker	UNP O60563
A	295	GLY	-	linker	UNP O60563
A	296	SER	-	linker	UNP O60563
A	297	GLY	-	linker	UNP O60563
A	298	GLY	-	linker	UNP O60563
A	299	GLY	-	linker	UNP O60563
A	300	THR	-	linker	UNP O60563
A	301	SER	-	linker	UNP O60563

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Chain	Residue	Modelled	Actual	Comment	Reference
B	77	ARG	GLN	SEE REMARK 999	UNP O60563
B	282	GLY	-	linker	UNP O60563
B	283	GLY	-	linker	UNP O60563
B	284	THR	-	linker	UNP O60563
B	285	GLY	-	linker	UNP O60563
B	286	GLY	-	linker	UNP O60563
B	287	GLY	-	linker	UNP O60563
B	288	SER	-	linker	UNP O60563
B	289	GLY	-	linker	UNP O60563
B	290	GLY	-	linker	UNP O60563
B	291	GLY	-	linker	UNP O60563
B	292	SER	-	linker	UNP O60563
B	293	GLY	-	linker	UNP O60563
B	294	GLY	-	linker	UNP O60563
B	295	GLY	-	linker	UNP O60563
B	296	SER	-	linker	UNP O60563
B	297	GLY	-	linker	UNP O60563
B	298	GLY	-	linker	UNP O60563
B	299	GLY	-	linker	UNP O60563
B	300	THR	-	linker	UNP O60563
B	301	SER	-	linker	UNP O60563
C	77	ARG	GLN	SEE REMARK 999	UNP O60563
C	282	GLY	-	linker	UNP O60563
C	283	GLY	-	linker	UNP O60563
C	284	THR	-	linker	UNP O60563
C	285	GLY	-	linker	UNP O60563
C	286	GLY	-	linker	UNP O60563
C	287	GLY	-	linker	UNP O60563
C	288	SER	-	linker	UNP O60563
C	289	GLY	-	linker	UNP O60563
C	290	GLY	-	linker	UNP O60563
C	291	GLY	-	linker	UNP O60563
C	292	SER	-	linker	UNP O60563
C	293	GLY	-	linker	UNP O60563
C	294	GLY	-	linker	UNP O60563
C	295	GLY	-	linker	UNP O60563
C	296	SER	-	linker	UNP O60563
C	297	GLY	-	linker	UNP O60563
C	298	GLY	-	linker	UNP O60563
C	299	GLY	-	linker	UNP O60563
C	300	THR	-	linker	UNP O60563
C	301	SER	-	linker	UNP O60563

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Chain	Residue	Modelled	Actual	Comment	Reference
D	77	ARG	GLN	SEE REMARK 999	UNP O60563
D	282	GLY	-	linker	UNP O60563
D	283	GLY	-	linker	UNP O60563
D	284	THR	-	linker	UNP O60563
D	285	GLY	-	linker	UNP O60563
D	286	GLY	-	linker	UNP O60563
D	287	GLY	-	linker	UNP O60563
D	288	SER	-	linker	UNP O60563
D	289	GLY	-	linker	UNP O60563
D	290	GLY	-	linker	UNP O60563
D	291	GLY	-	linker	UNP O60563
D	292	SER	-	linker	UNP O60563
D	293	GLY	-	linker	UNP O60563
D	294	GLY	-	linker	UNP O60563
D	295	GLY	-	linker	UNP O60563
D	296	SER	-	linker	UNP O60563
D	297	GLY	-	linker	UNP O60563
D	298	GLY	-	linker	UNP O60563
D	299	GLY	-	linker	UNP O60563
D	300	THR	-	linker	UNP O60563
D	301	SER	-	linker	UNP O60563

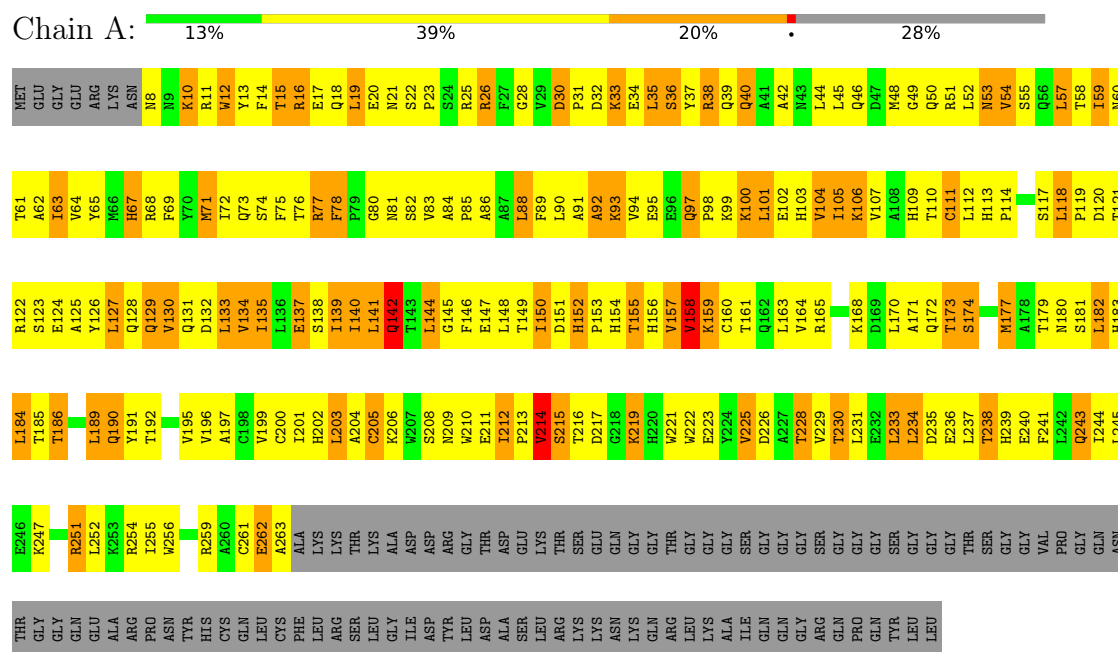
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	25	Total O 25 25	0	0
2	B	16	Total O 16 16	0	0
2	C	21	Total O 21 21	0	0
2	D	17	Total O 17 17	0	0

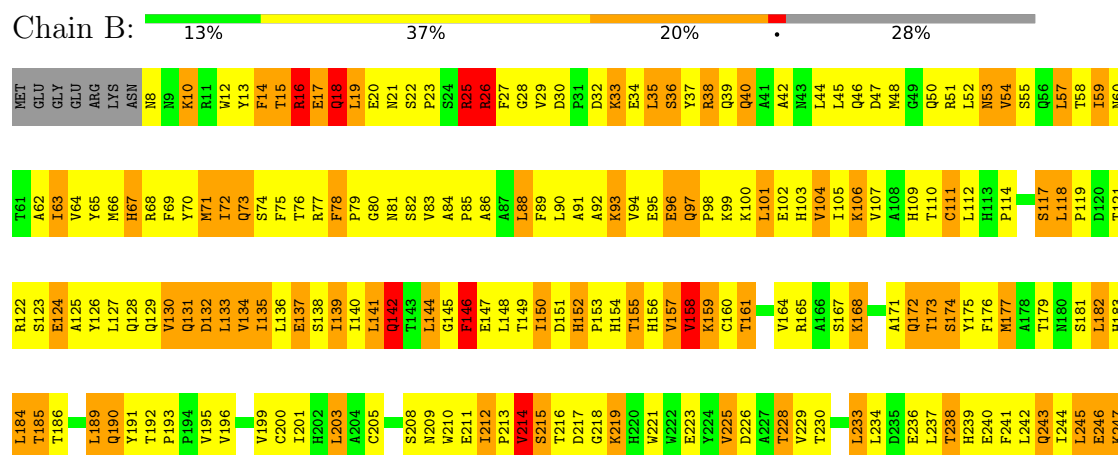
3 Residue-property plots

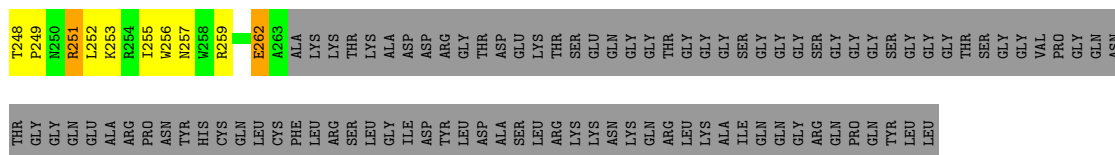
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cyclin-T1, Protein Tat

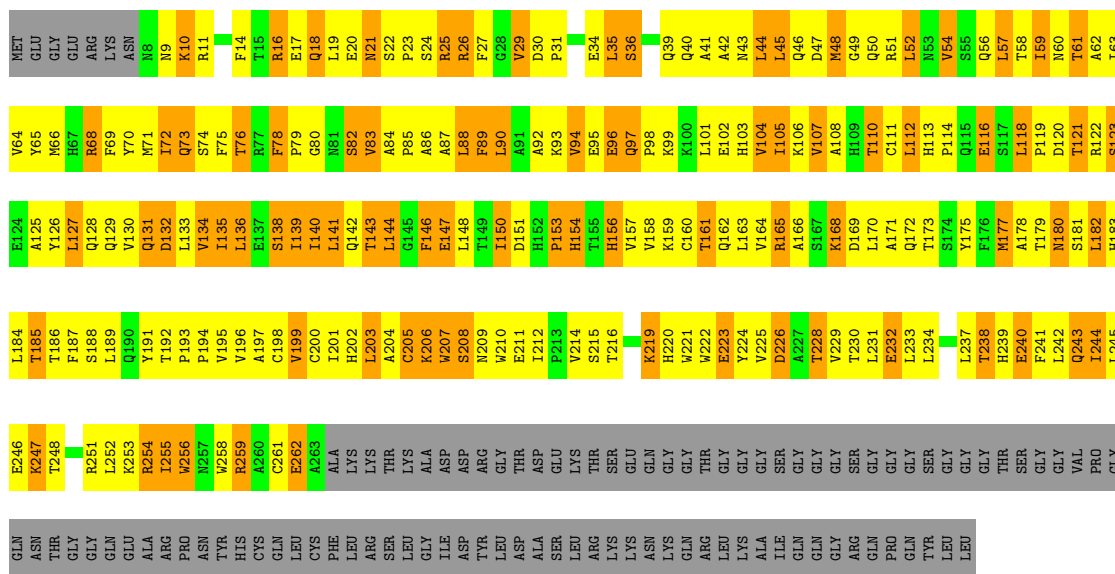
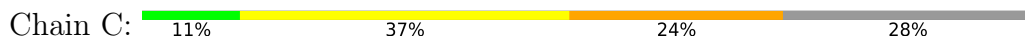


• Molecule 1: Cyclin-T1, Protein Tat

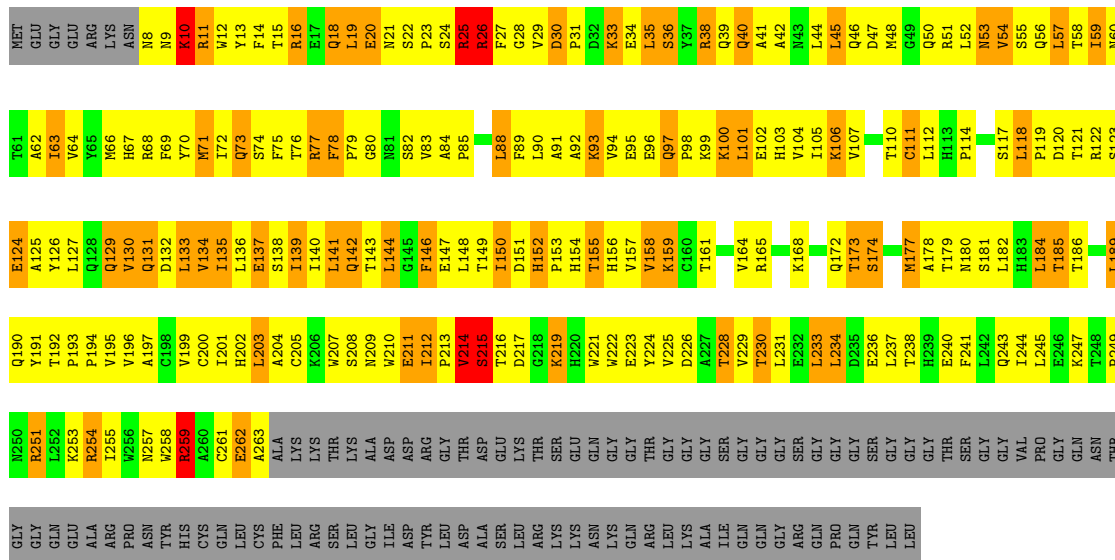




- Molecule 1: Cyclin-T1, Protein Tat



- Molecule 1: Cyclin-T1, Protein Tat



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	203.83Å 203.83Å 124.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.67 50.00 – 2.67	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.67) 99.7 (50.00-2.67)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.67Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.274 , 0.306 0.248 , 0.271	Depositor DCC
R_{free} test set	1548 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 91.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.188 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.186 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.186 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.437 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.438 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.430 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.187 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.39	1/2130 (0.0%)	0.98	2/2904 (0.1%)
1	B	0.36	0/2134	1.08	14/2909 (0.5%)
1	C	0.30	0/2136	0.95	2/2911 (0.1%)
1	D	0.37	0/2133	1.03	12/2908 (0.4%)
All	All	0.36	1/8533 (0.0%)	1.01	30/11632 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	GLN	CD-OE1	5.75	1.34	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	GLN	CA-C-N	9.25	138.35	121.70
1	B	18	GLN	C-N-CA	9.25	138.35	121.70
1	D	142	GLN	CG-CD-NE2	8.30	128.84	116.40
1	B	16	ARG	CA-C-N	8.28	136.60	121.70
1	B	16	ARG	C-N-CA	8.28	136.60	121.70
1	D	259	ARG	CA-CB-CG	7.80	129.70	114.10
1	B	25	ARG	CA-C-N	6.92	130.48	120.38
1	B	25	ARG	C-N-CA	6.92	130.48	120.38
1	B	146	PHE	CA-CB-CG	6.63	120.43	113.80
1	B	142	GLN	OE1-CD-NE2	6.49	129.09	122.60
1	B	214	VAL	CA-C-N	6.43	130.89	121.31
1	B	214	VAL	C-N-CA	6.43	130.89	121.31
1	D	100	LYS	CB-CG-CD	6.34	125.89	111.30
1	A	214	VAL	CA-C-N	6.34	130.75	121.31
1	A	214	VAL	C-N-CA	6.34	130.75	121.31
1	C	175	TYR	CA-C-N	6.25	131.15	120.72
1	C	175	TYR	C-N-CA	6.25	131.15	120.72
1	D	214	VAL	CA-C-N	6.05	133.09	121.54
1	D	214	VAL	C-N-CA	6.05	133.09	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	ARG	CD-NE-CZ	5.96	132.75	124.40
1	D	25	ARG	O-C-N	5.74	128.29	122.09
1	D	146	PHE	CA-CB-CG	5.69	119.49	113.80
1	D	212	ILE	N-CA-C	5.68	112.73	107.56
1	B	18	GLN	N-CA-C	5.32	116.89	111.14
1	D	142	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	D	26	ARG	CG-CD-NE	5.16	123.36	112.00
1	D	26	ARG	CD-NE-CZ	5.11	131.55	124.40
1	B	17	GLU	CA-C-N	5.11	127.38	120.44
1	B	17	GLU	C-N-CA	5.11	127.38	120.44
1	D	100	LYS	CG-CD-CE	5.04	122.89	111.30

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	2076	0	2043	264	0
1	B	2080	0	2045	246	0
1	C	2082	0	2052	323	0
1	D	2079	0	2045	229	0
2	A	25	0	0	6	0
2	B	16	0	0	4	0
2	C	21	0	0	3	0
2	D	17	0	0	0	0
All	All	8396	0	8185	1023	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 62.

All (1023) 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:15:THR:HG23	1:A:18:GLN:HB2	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:SER:HG	1:D:224:TYR:HE1	1.04	1.02
1:A:177:MET:HB3	1:A:200:CYS:HB3	1.42	0.98
1:C:63:ILE:HG21	1:C:182:LEU:HB3	1.47	0.97
1:C:239:HIS:HA	1:C:242:LEU:HD12	1.47	0.97
1:D:214:VAL:HG21	1:D:221:TRP:HB3	1.46	0.96
1:B:259:ARG:HA	1:B:262:GLU:HG3	1.44	0.96
1:C:136:LEU:HA	1:C:139:ILE:HG13	1.45	0.96
1:D:105:ILE:HD11	1:D:133:LEU:HG	1.46	0.95
1:C:16:ARG:HH21	1:C:19:LEU:HD13	1.30	0.94
1:D:45:LEU:HD13	1:D:63:ILE:HD13	1.48	0.94
1:B:138:SER:HA	1:B:141:LEU:HB2	1.50	0.93
1:D:52:LEU:HG	1:D:107:VAL:HG21	1.50	0.93
1:B:92:ALA:HB1	1:B:98:PRO:HA	1.52	0.90
1:B:151:ASP:HB2	1:B:193:PRO:HG2	1.51	0.90
1:B:118:LEU:HG	1:B:119:PRO:HD2	1.52	0.90
1:A:45:LEU:HD21	1:A:62:ALA:HB3	1.54	0.89
1:C:50:GLN:HG3	1:C:59:ILE:HD11	1.54	0.88
1:A:177:MET:HE2	1:A:203:LEU:HD22	1.56	0.88
1:D:177:MET:HE2	1:D:203:LEU:HD22	1.56	0.88
1:D:118:LEU:HG	1:D:119:PRO:HD2	1.57	0.87
1:B:14:PHE:HE2	1:B:189:LEU:HB3	1.39	0.87
1:C:197:ALA:HB3	1:C:225:VAL:HG11	1.55	0.87
1:B:23:PRO:HA	1:B:26:ARG:HG3	1.57	0.86
1:A:21:ASN:HA	1:A:25:ARG:HG2	1.54	0.86
1:A:140:ILE:HG12	1:A:144:LEU:HD11	1.56	0.85
1:D:29:VAL:HG12	1:D:33:LYS:HB3	1.58	0.85
1:A:74:SER:HB3	1:A:77:ARG:HG3	1.57	0.85
1:D:185:THR:HG22	1:D:244:ILE:HG21	1.59	0.85
1:C:25:ARG:HB2	1:C:25:ARG:HH21	1.41	0.84
1:C:157:VAL:HG23	1:C:197:ALA:HB1	1.59	0.84
1:A:16:ARG:HD3	1:B:233:LEU:HD11	1.59	0.83
1:D:92:ALA:HB1	1:D:98:PRO:HA	1.57	0.83
1:B:233:LEU:HA	1:B:236:GLU:HB3	1.58	0.82
1:C:228:THR:HG21	1:D:21:ASN:HB2	1.58	0.82
1:C:253:LYS:HA	1:C:256:TRP:HB2	1.62	0.82
1:A:45:LEU:HD13	1:A:63:ILE:HD13	1.62	0.82
1:C:177:MET:HG3	1:C:241:PHE:HE1	1.43	0.82
1:C:9:ASN:OD1	1:C:11:ARG:HG2	1.80	0.81
1:A:137:GLU:HG3	1:A:141:LEU:HD12	1.62	0.81
1:B:226:ASP:HB3	1:B:229:VAL:HG23	1.63	0.81
1:C:48:MET:HA	1:C:51:ARG:HD2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ASP:HB3	1:D:229:VAL:HG23	1.64	0.80
1:C:136:LEU:O	1:C:140:ILE:HG22	1.80	0.80
1:A:157:VAL:HG22	1:A:201:ILE:HD11	1.64	0.80
1:C:54:VAL:HG13	1:C:58:THR:HB	1.65	0.79
1:A:118:LEU:HG	1:A:119:PRO:HD2	1.65	0.79
1:A:225:VAL:HG22	2:A:372:HOH:O	1.82	0.79
1:B:135:ILE:O	1:B:139:ILE:HD13	1.83	0.79
1:C:16:ARG:HD2	1:D:233:LEU:HD13	1.65	0.78
1:D:135:ILE:O	1:D:139:ILE:HD13	1.84	0.78
1:D:140:ILE:HG12	1:D:144:LEU:HD11	1.65	0.78
1:B:192:THR:O	1:B:196:VAL:HG23	1.84	0.78
1:A:233:LEU:O	1:A:237:LEU:HG	1.84	0.78
1:D:80:GLY:HA2	1:D:83:VAL:HB	1.66	0.77
1:A:58:THR:HA	1:A:95:GLU:HG3	1.66	0.77
1:C:41:ALA:O	1:C:45:LEU:HD12	1.85	0.77
1:A:105:ILE:HG12	1:A:133:LEU:HD12	1.65	0.77
1:A:138:SER:OG	1:D:138:SER:HB2	1.85	0.77
1:C:90:LEU:HA	1:C:93:LYS:HG2	1.66	0.77
1:A:90:LEU:HD21	1:A:141:LEU:HA	1.66	0.76
1:A:135:ILE:O	1:A:139:ILE:HD13	1.85	0.76
1:A:82:SER:O	1:A:85:PRO:HD2	1.86	0.76
1:C:46:GLN:OE1	1:C:59:ILE:HG21	1.85	0.76
1:C:16:ARG:HA	1:C:19:LEU:HB2	1.66	0.76
1:D:66:MET:HG2	1:D:70:TYR:HE2	1.51	0.76
1:B:101:LEU:O	1:B:105:ILE:HG13	1.86	0.75
1:D:236:GLU:HG2	1:D:237:LEU:HD23	1.66	0.75
1:C:194:PRO:HB3	1:C:225:VAL:O	1.86	0.75
1:D:16:ARG:HH21	1:D:190:GLN:HE21	1.33	0.74
1:D:15:THR:OG1	1:D:18:GLN:HB2	1.86	0.74
1:A:252:LEU:HA	1:A:255:ILE:HD12	1.69	0.74
1:B:79:PRO:O	1:B:83:VAL:HG23	1.88	0.74
1:B:64:VAL:O	1:B:68:ARG:HD2	1.88	0.74
1:B:239:HIS:O	1:B:243:GLN:HB2	1.87	0.74
1:C:128:GLN:HA	1:C:131:GLN:HB2	1.68	0.74
1:A:101:LEU:O	1:A:105:ILE:HG13	1.88	0.73
1:A:12:TRP:HB3	1:A:68:ARG:HE	1.51	0.73
1:C:240:GLU:O	1:C:243:GLN:HB2	1.89	0.73
1:C:68:ARG:O	1:C:71:MET:HB2	1.87	0.73
1:C:198:CYS:O	1:C:202:HIS:HB2	1.88	0.72
1:A:127:LEU:O	1:A:130:VAL:HB	1.90	0.72
1:C:112:LEU:HD12	2:C:374:HOH:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ARG:NH2	1:D:190:GLN:HE21	1.87	0.72
1:C:188:SER:OG	1:C:189:LEU:HD12	1.90	0.72
1:A:25:ARG:NH2	1:A:31:PRO:HA	2.05	0.72
1:B:126:TYR:O	1:B:130:VAL:HG23	1.89	0.72
1:A:170:LEU:HD13	1:A:208:SER:OG	1.90	0.71
1:C:16:ARG:NH2	1:C:19:LEU:HD13	2.04	0.71
1:A:12:TRP:HB3	1:A:68:ARG:NE	2.04	0.71
1:D:41:ALA:O	1:D:45:LEU:HD12	1.90	0.71
1:A:90:LEU:HA	1:A:93:LYS:NZ	2.04	0.71
1:A:251:ARG:HD3	1:A:254:ARG:HE	1.54	0.71
1:B:90:LEU:HD21	1:B:141:LEU:HG	1.71	0.71
1:B:48:MET:HG2	1:B:107:VAL:HG12	1.72	0.71
1:B:52:LEU:HD22	1:B:99:LYS:HG3	1.73	0.71
1:B:127:LEU:O	1:B:130:VAL:HB	1.91	0.71
1:C:17:GLU:O	1:C:21:ASN:HB2	1.91	0.71
1:D:79:PRO:O	1:D:83:VAL:HG23	1.89	0.71
1:B:80:GLY:HA2	1:B:83:VAL:HB	1.73	0.71
1:D:54:VAL:HG13	1:D:58:THR:HB	1.72	0.71
1:B:245:LEU:O	1:B:252:LEU:HB2	1.91	0.71
1:B:55:SER:OG	1:B:57:LEU:HD23	1.91	0.70
1:D:106:LYS:HE2	1:D:119:PRO:HG2	1.73	0.70
1:B:247:LYS:O	1:B:249:PRO:HD3	1.90	0.70
1:B:242:LEU:HA	1:B:245:LEU:HD12	1.73	0.70
1:C:25:ARG:HD2	1:C:31:PRO:HG3	1.74	0.70
1:C:244:ILE:H	1:C:244:ILE:HD12	1.54	0.70
1:B:36:SER:O	1:B:40:GLN:HB2	1.92	0.70
1:A:91:ALA:O	1:A:95:GLU:HG2	1.92	0.70
1:C:245:LEU:O	1:C:252:LEU:HD13	1.92	0.70
1:A:145:GLY:HA2	1:D:142:GLN:OE1	1.91	0.70
1:C:118:LEU:HD22	1:C:119:PRO:HD3	1.74	0.70
1:C:132:ASP:O	1:C:135:ILE:HG22	1.91	0.69
1:A:22:SER:O	1:A:25:ARG:HB2	1.92	0.69
1:C:10:LYS:HD2	1:D:18:GLN:NE2	2.07	0.69
1:C:62:ALA:HA	1:C:65:TYR:HB2	1.73	0.69
1:A:180:ASN:O	1:A:184:LEU:HB2	1.92	0.69
1:C:159:LYS:O	1:C:163:LEU:HD12	1.92	0.69
1:C:244:ILE:O	1:C:248:THR:HG23	1.91	0.69
1:D:192:THR:O	1:D:196:VAL:HG23	1.91	0.69
1:A:103:HIS:O	1:A:107:VAL:HG23	1.92	0.69
1:A:219:LYS:NZ	1:A:223:GLU:HB3	2.07	0.69
1:D:64:VAL:HG11	1:D:150:ILE:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLU:O	1:A:106:LYS:HB2	1.93	0.69
1:C:56:GLN:HG3	1:C:60:ASN:HD21	1.57	0.69
1:A:60:ASN:O	1:A:64:VAL:HG23	1.92	0.69
1:A:80:GLY:HA2	2:A:370:HOH:O	1.92	0.69
1:A:83:VAL:HB	2:A:370:HOH:O	1.92	0.69
1:A:160:CYS:O	1:A:164:VAL:HG22	1.92	0.69
1:D:36:SER:O	1:D:40:GLN:HB2	1.93	0.69
1:C:183:HIS:O	1:C:184:LEU:HD23	1.93	0.68
1:D:156:HIS:HA	1:D:159:LYS:HD2	1.76	0.68
1:C:85:PRO:O	1:C:89:PHE:HB2	1.93	0.68
1:A:61:THR:O	1:A:64:VAL:HB	1.92	0.68
1:B:19:LEU:HD11	1:B:38:ARG:HH21	1.58	0.68
1:B:103:HIS:HA	1:B:106:LYS:HB2	1.75	0.68
1:C:133:LEU:HA	1:C:136:LEU:HG	1.76	0.68
1:D:101:LEU:HD21	1:D:133:LEU:HB3	1.74	0.68
1:A:35:LEU:O	1:A:39:GLN:HG3	1.94	0.68
1:B:14:PHE:CE2	1:B:189:LEU:HB3	2.27	0.67
1:D:217:ASP:OD2	1:D:219:LYS:HB2	1.94	0.67
1:B:123:SER:O	1:B:127:LEU:HG	1.95	0.67
1:C:51:ARG:HH11	1:C:107:VAL:HG13	1.60	0.67
1:C:261:CYS:SG	1:C:261:CYS:O	2.52	0.67
1:D:258:TRP:O	1:D:262:GLU:HB2	1.93	0.67
1:A:48:MET:HE2	1:A:88:LEU:HD23	1.77	0.67
1:D:152:HIS:HB3	1:D:154:HIS:ND1	2.09	0.67
1:C:230:THR:HG22	1:C:233:LEU:HB3	1.76	0.67
1:A:16:ARG:NH1	1:B:237:LEU:HD21	2.10	0.66
1:D:211:GLU:O	1:D:213:PRO:HD3	1.96	0.66
1:B:139:ILE:HD12	1:C:146:PHE:HZ	1.61	0.66
1:C:105:ILE:HD11	1:C:133:LEU:HD13	1.77	0.66
1:A:100:LYS:HD3	1:A:103:HIS:HB2	1.77	0.66
1:D:251:ARG:HH11	1:D:254:ARG:HB3	1.60	0.66
1:C:192:THR:O	1:C:196:VAL:HG23	1.95	0.66
1:B:85:PRO:HB3	1:B:104:VAL:HG13	1.78	0.66
1:B:246:GLU:O	1:B:247:LYS:HD3	1.95	0.66
1:B:212:ILE:O	1:B:214:VAL:HG22	1.95	0.65
1:B:233:LEU:O	1:B:237:LEU:HG	1.96	0.65
1:C:47:ASP:O	1:C:51:ARG:HG3	1.96	0.65
1:B:45:LEU:HD21	1:B:62:ALA:HB3	1.78	0.65
1:A:228:THR:HG22	1:B:21:ASN:HD22	1.61	0.65
1:B:19:LEU:HD21	1:B:71:MET:SD	2.37	0.65
1:B:60:ASN:O	1:B:64:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLN:O	1:C:50:GLN:HB2	1.96	0.65
1:C:78:PHE:HZ	1:C:139:ILE:HG21	1.62	0.65
1:C:93:LYS:HA	1:C:98:PRO:HB3	1.77	0.65
1:C:180:ASN:ND2	1:C:180:ASN:H	1.94	0.65
1:D:124:GLU:OE1	1:D:124:GLU:HA	1.95	0.65
1:A:173:THR:HB	1:A:204:ALA:HB1	1.77	0.65
1:B:14:PHE:HB2	1:B:17:GLU:HB3	1.78	0.65
1:D:55:SER:OG	1:D:57:LEU:HD23	1.96	0.65
1:B:96:GLU:HA	1:B:96:GLU:OE1	1.97	0.64
1:B:39:GLN:HA	1:B:183:HIS:O	1.97	0.64
1:B:252:LEU:O	1:B:255:ILE:HB	1.96	0.64
1:B:152:HIS:HB3	1:B:154:HIS:ND1	2.11	0.64
1:B:82:SER:O	1:B:85:PRO:HD2	1.97	0.64
1:A:30:ASP:HB2	1:A:33:LYS:HB2	1.80	0.64
1:C:207:TRP:HH2	1:C:255:ILE:HG22	1.62	0.64
1:B:68:ARG:HA	1:B:71:MET:HG3	1.79	0.64
1:C:107:VAL:HA	1:C:110:THR:OG1	1.97	0.64
1:D:12:TRP:HH2	1:D:144:LEU:HA	1.63	0.64
1:B:38:ARG:HH12	1:B:189:LEU:HD11	1.63	0.64
1:C:220:HIS:HB2	1:C:223:GLU:OE2	1.97	0.64
1:A:212:ILE:O	1:A:214:VAL:HG22	1.97	0.63
1:C:199:VAL:HG12	1:C:238:THR:HB	1.80	0.63
1:A:259:ARG:HA	1:A:262:GLU:HG3	1.78	0.63
1:C:140:ILE:O	1:C:144:LEU:HG	1.98	0.63
1:D:70:TYR:OH	1:D:83:VAL:HG11	1.98	0.63
1:C:16:ARG:HA	1:C:19:LEU:HD12	1.81	0.63
1:D:23:PRO:HA	1:D:26:ARG:HD3	1.79	0.63
1:B:154:HIS:HB3	1:B:175:TYR:CE1	2.34	0.63
1:A:237:LEU:O	1:A:241:PHE:HB2	1.99	0.63
1:A:21:ASN:HB2	1:B:228:THR:HB	1.81	0.63
1:C:153:PRO:HB3	1:C:193:PRO:O	1.99	0.63
1:C:191:TYR:CD1	1:C:237:LEU:HD11	2.33	0.63
1:C:166:ALA:HB3	1:C:171:ALA:HB2	1.81	0.63
1:A:203:LEU:HD12	1:A:238:THR:HA	1.80	0.62
1:D:253:LYS:HG2	1:D:257:ASN:HD21	1.63	0.62
1:A:112:LEU:O	1:A:114:PRO:HD3	1.99	0.62
1:A:179:THR:HG23	1:A:183:HIS:CE1	2.34	0.62
1:A:252:LEU:O	1:A:255:ILE:HB	2.00	0.62
1:B:10:LYS:O	1:B:10:LYS:HG3	1.99	0.62
1:B:246:GLU:OE1	1:B:246:GLU:HA	1.99	0.62
1:C:222:TRP:HB2	1:C:229:VAL:HG11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:SER:O	1:D:85:PRO:HD2	1.99	0.62
1:D:253:LYS:HG2	1:D:257:ASN:ND2	2.13	0.62
1:A:49:GLY:HA3	1:A:59:ILE:HD11	1.82	0.62
1:B:21:ASN:HD21	1:B:26:ARG:HH22	1.46	0.62
1:C:192:THR:HG23	1:C:194:PRO:HD2	1.81	0.62
1:A:68:ARG:NH1	1:A:150:ILE:HD11	2.13	0.62
1:A:94:VAL:HG22	1:A:148:LEU:HD23	1.82	0.62
1:C:49:GLY:O	1:C:54:VAL:HB	2.00	0.62
1:D:68:ARG:HA	1:D:189:LEU:HD21	1.79	0.62
1:C:222:TRP:O	1:C:229:VAL:HB	2.00	0.62
1:D:140:ILE:O	1:D:144:LEU:HG	2.00	0.62
1:D:207:TRP:HH2	1:D:255:ILE:HG22	1.65	0.62
1:C:153:PRO:HB3	1:C:193:PRO:HA	1.82	0.62
1:D:91:ALA:O	1:D:95:GLU:HG2	2.00	0.62
1:D:103:HIS:O	1:D:107:VAL:HG23	1.99	0.62
1:D:247:LYS:O	1:D:249:PRO:HD3	1.99	0.62
1:A:13:TYR:HB3	1:B:15:THR:HG21	1.81	0.61
1:A:48:MET:HG3	1:A:111:CYS:SG	2.40	0.61
1:C:120:ASP:HB3	1:C:123:SER:HB2	1.81	0.61
1:A:85:PRO:HB2	1:A:133:LEU:HD11	1.82	0.61
1:C:191:TYR:CE2	1:C:237:LEU:HD21	2.35	0.61
1:C:192:THR:OG1	1:C:194:PRO:HD2	2.00	0.61
1:C:21:ASN:O	1:C:26:ARG:HD3	2.00	0.61
1:A:240:GLU:O	1:A:244:ILE:HG12	2.01	0.61
1:B:124:GLU:OE1	1:B:124:GLU:HA	1.99	0.61
1:C:72:ILE:HD12	1:C:143:THR:HG22	1.83	0.61
1:D:48:MET:HA	1:D:111:CYS:SG	2.40	0.61
1:A:219:LYS:HZ2	1:A:223:GLU:HB3	1.63	0.61
1:D:35:LEU:O	1:D:39:GLN:HG3	2.00	0.61
1:A:214:VAL:HG12	1:A:215:SER:H	1.65	0.61
1:B:54:VAL:HG13	1:B:58:THR:HB	1.82	0.61
1:B:16:ARG:HA	1:B:18:GLN:N	2.16	0.61
1:D:215:SER:HB2	1:D:217:ASP:OD1	2.00	0.61
1:C:179:THR:O	1:C:183:HIS:HD2	1.83	0.61
1:D:93:LYS:N	1:D:98:PRO:HB3	2.16	0.61
1:D:240:GLU:O	1:D:244:ILE:HG12	2.00	0.61
1:A:55:SER:HB3	1:A:58:THR:OG1	2.00	0.60
1:C:59:ILE:O	1:C:63:ILE:HG12	2.01	0.60
1:D:231:LEU:HA	1:D:234:LEU:HB2	1.82	0.60
1:B:243:GLN:HA	1:B:246:GLU:HB2	1.82	0.60
1:D:233:LEU:HA	1:D:236:GLU:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:TYR:HB3	1:B:75:PHE:CD1	2.36	0.60
1:B:40:GLN:HG2	2:B:363:HOH:O	2.00	0.60
1:C:46:GLN:O	1:C:46:GLN:HG3	2.00	0.60
1:A:145:GLY:HA2	1:D:142:GLN:HE22	1.67	0.60
1:C:215:SER:HB2	1:C:219:LYS:HB2	1.84	0.60
1:C:199:VAL:HG13	1:C:234:LEU:HD12	1.82	0.60
1:D:64:VAL:O	1:D:68:ARG:HD2	2.02	0.60
1:A:90:LEU:HD11	1:A:141:LEU:HG	1.83	0.59
1:B:73:GLN:HB3	1:B:78:PHE:CE2	2.37	0.59
1:B:107:VAL:O	1:B:111:CYS:HB2	2.02	0.59
1:A:154:HIS:O	1:A:158:VAL:HG23	2.02	0.59
1:B:139:ILE:HD12	1:C:146:PHE:CZ	2.36	0.59
1:B:185:THR:HG22	1:B:244:ILE:HG21	1.85	0.59
1:C:20:GLU:HA	1:C:25:ARG:HG2	1.84	0.59
1:C:42:ALA:HA	1:C:45:LEU:CD1	2.32	0.59
1:D:90:LEU:O	1:D:94:VAL:HG23	2.02	0.59
1:A:146:PHE:HZ	1:D:139:ILE:HA	1.66	0.59
1:C:96:GLU:O	1:C:98:PRO:HD3	2.03	0.59
1:B:65:TYR:HB3	1:B:140:ILE:HD11	1.83	0.59
1:B:109:HIS:CG	1:B:119:PRO:HD3	2.38	0.59
1:B:167:SER:O	1:B:171:ALA:HB2	2.03	0.59
1:D:16:ARG:HD2	1:D:16:ARG:N	2.18	0.59
1:B:39:GLN:HG2	1:B:184:LEU:O	2.03	0.59
1:A:71:MET:SD	1:A:189:LEU:HD22	2.43	0.59
1:A:92:ALA:HB1	1:A:98:PRO:HA	1.83	0.59
1:A:155:THR:O	1:A:159:LYS:HG3	2.03	0.59
1:D:14:PHE:CE1	1:D:71:MET:HE2	2.37	0.59
1:B:8:ASN:N	1:B:13:TYR:HH	2.00	0.59
1:C:191:TYR:CZ	1:C:237:LEU:HD21	2.38	0.59
1:B:52:LEU:HG	1:B:107:VAL:HG21	1.84	0.58
1:C:132:ASP:O	1:C:136:LEU:HD23	2.03	0.58
1:D:153:PRO:HB3	1:D:196:VAL:HB	1.85	0.58
1:A:39:GLN:HB2	2:A:366:HOH:O	2.04	0.58
1:B:46:GLN:O	1:B:50:GLN:HG3	2.03	0.58
1:C:54:VAL:HG22	1:C:58:THR:HG21	1.85	0.58
1:A:14:PHE:CZ	1:A:71:MET:HE2	2.39	0.58
1:B:192:THR:OG1	1:B:195:VAL:HG23	2.04	0.58
1:A:259:ARG:HA	1:A:262:GLU:OE2	2.04	0.58
1:B:91:ALA:O	1:B:95:GLU:HG2	2.03	0.58
1:A:146:PHE:O	1:A:148:LEU:HD12	2.04	0.58
1:B:102:GLU:O	1:B:106:LYS:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:MET:HG2	1:B:107:VAL:CG1	2.33	0.58
1:D:46:GLN:OE1	1:D:59:ILE:HG21	2.04	0.58
1:A:236:GLU:HG2	1:A:237:LEU:HD23	1.84	0.58
1:B:19:LEU:CD1	1:B:38:ARG:HH21	2.16	0.58
1:B:214:VAL:HG12	1:B:215:SER:H	1.68	0.58
1:C:90:LEU:CD2	1:C:141:LEU:HG	2.34	0.58
1:A:126:TYR:O	1:A:130:VAL:HG23	2.03	0.58
1:A:222:TRP:CZ2	1:A:231:LEU:HD22	2.39	0.58
1:C:16:ARG:HG3	1:C:16:ARG:O	2.03	0.58
1:A:94:VAL:HG22	1:A:148:LEU:CD2	2.33	0.57
1:C:23:PRO:O	1:C:27:PHE:HB2	2.04	0.57
1:C:178:ALA:O	1:C:182:LEU:HD22	2.03	0.57
1:B:134:VAL:HG11	1:C:135:ILE:HG12	1.86	0.57
1:C:160:CYS:O	1:C:164:VAL:HG13	2.03	0.57
1:A:137:GLU:O	1:A:141:LEU:HB2	2.04	0.57
1:A:191:TYR:CE1	1:B:16:ARG:HD2	2.39	0.57
1:C:40:GLN:O	1:C:44:LEU:HD22	2.05	0.57
1:A:228:THR:CG2	1:B:21:ASN:HD22	2.16	0.57
1:B:45:LEU:HD21	1:B:62:ALA:CB	2.34	0.57
1:D:12:TRP:CE3	1:D:68:ARG:HG2	2.40	0.57
1:C:84:ALA:O	1:C:88:LEU:HB2	2.04	0.57
1:C:180:ASN:O	1:C:184:LEU:HG	2.04	0.57
1:A:179:THR:O	1:A:183:HIS:HB2	2.05	0.57
1:C:177:MET:HG2	1:C:203:LEU:HB2	1.86	0.57
1:C:179:THR:O	1:C:182:LEU:HB2	2.04	0.57
1:D:259:ARG:O	1:D:259:ARG:HG3	2.04	0.57
1:A:157:VAL:HG22	1:A:201:ILE:CD1	2.34	0.57
1:B:19:LEU:HD13	1:B:22:SER:OG	2.04	0.57
1:B:134:VAL:CG1	1:C:135:ILE:HG12	2.35	0.57
1:D:223:GLU:HA	1:D:226:ASP:O	2.04	0.57
1:A:174:SER:HB3	1:A:201:ILE:HD13	1.86	0.57
1:B:19:LEU:HD22	1:B:22:SER:OG	2.05	0.57
1:C:90:LEU:HD21	1:C:141:LEU:HG	1.87	0.57
1:A:211:GLU:O	1:A:213:PRO:HD3	2.05	0.56
1:A:228:THR:HG21	1:B:21:ASN:HB2	1.86	0.56
1:B:156:HIS:HB3	1:B:225:VAL:CG1	2.35	0.56
1:C:112:LEU:O	1:C:114:PRO:HD3	2.05	0.56
1:C:130:VAL:O	1:C:134:VAL:HB	2.04	0.56
1:D:106:LYS:CE	1:D:119:PRO:HG2	2.35	0.56
1:A:239:HIS:O	1:A:243:GLN:HB2	2.05	0.56
1:B:39:GLN:HE21	1:B:184:LEU:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:ARG:HD2	1:D:255:ILE:HG13	1.87	0.56
1:A:45:LEU:HD21	1:A:62:ALA:CB	2.31	0.56
1:A:210:TRP:CD1	1:A:211:GLU:H	2.23	0.56
1:B:184:LEU:HD12	1:B:245:LEU:HD23	1.87	0.56
1:C:54:VAL:HG11	1:C:59:ILE:HG13	1.87	0.56
1:C:121:THR:HA	1:C:126:TYR:CD2	2.41	0.56
1:D:58:THR:HG23	1:D:95:GLU:HG3	1.86	0.56
1:D:233:LEU:HD12	1:D:236:GLU:OE2	2.05	0.56
1:B:240:GLU:O	1:B:244:ILE:HG12	2.04	0.56
1:C:156:HIS:HB2	1:C:225:VAL:HG13	1.88	0.56
1:C:177:MET:HG3	1:C:241:PHE:CE1	2.34	0.56
1:A:177:MET:HE2	1:A:203:LEU:CD2	2.33	0.56
1:B:66:MET:HG2	1:B:70:TYR:HE2	1.69	0.56
1:A:251:ARG:NE	1:A:254:ARG:HH21	2.03	0.56
1:C:27:PHE:CD2	1:C:76:THR:HG21	2.41	0.56
1:C:205:CYS:HB3	1:C:210:TRP:O	2.05	0.56
1:A:69:PHE:HD1	1:A:140:ILE:HG13	1.70	0.56
1:C:24:SER:HG	1:C:75:PHE:HD2	1.54	0.56
1:D:127:LEU:O	1:D:130:VAL:HB	2.05	0.56
1:D:190:GLN:HB3	1:D:191:TYR:CE2	2.41	0.56
1:D:42:ALA:HA	1:D:45:LEU:HD12	1.88	0.56
1:D:177:MET:HE3	1:D:241:PHE:CZ	2.41	0.55
1:A:90:LEU:HD21	1:A:141:LEU:CA	2.36	0.55
1:C:197:ALA:CB	1:C:225:VAL:HG11	2.34	0.55
1:D:10:LYS:NZ	1:D:10:LYS:HB3	2.18	0.55
1:A:262:GLU:O	1:A:263:ALA:O	2.24	0.55
1:B:22:SER:O	1:B:25:ARG:HB2	2.06	0.55
1:C:136:LEU:CA	1:C:139:ILE:HG13	2.30	0.55
1:D:66:MET:HG2	1:D:70:TYR:CE2	2.39	0.55
1:D:44:LEU:HG	1:D:48:MET:SD	2.47	0.55
1:A:171:ALA:HA	1:A:174:SER:OG	2.06	0.55
1:D:222:TRP:HB2	1:D:229:VAL:HG11	1.89	0.55
1:C:120:ASP:HB3	1:C:123:SER:CB	2.36	0.55
1:B:68:ARG:HG3	1:B:189:LEU:CD2	2.36	0.55
1:A:145:GLY:HA2	1:D:142:GLN:NE2	2.22	0.55
1:C:56:GLN:HE22	1:C:59:ILE:CG2	2.20	0.55
1:C:221:TRP:O	1:C:224:TYR:HD1	1.90	0.55
1:B:67:HIS:HB3	1:B:189:LEU:HD11	1.89	0.55
1:B:164:VAL:O	1:B:165:ARG:HB2	2.07	0.55
1:C:42:ALA:HB2	1:C:66:MET:HE1	1.89	0.55
1:B:16:ARG:CG	1:B:18:GLN:HG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ARG:HH22	1:B:34:GLU:HB3	1.72	0.54
1:C:113:HIS:HB3	1:C:116:GLU:HB2	1.89	0.54
1:C:192:THR:OG1	1:C:193:PRO:HD2	2.07	0.54
1:D:70:TYR:OH	1:D:83:VAL:HG21	2.07	0.54
1:D:126:TYR:O	1:D:130:VAL:HG23	2.07	0.54
1:A:90:LEU:HA	1:A:93:LYS:HZ3	1.70	0.54
1:C:132:ASP:O	1:C:136:LEU:CD2	2.56	0.54
1:C:156:HIS:HA	1:C:159:LYS:HB3	1.88	0.54
1:A:105:ILE:HD11	1:A:133:LEU:HB2	1.90	0.54
1:C:199:VAL:HG13	1:C:234:LEU:CD1	2.37	0.54
1:C:222:TRP:CZ2	1:C:231:LEU:HB2	2.41	0.54
1:B:190:GLN:HB3	1:B:191:TYR:CD2	2.43	0.54
1:B:35:LEU:O	1:B:39:GLN:HG3	2.07	0.54
1:C:118:LEU:HD13	1:C:119:PRO:HD2	1.90	0.54
1:D:102:GLU:O	1:D:106:LYS:HB2	2.07	0.54
1:A:164:VAL:HB	1:A:212:ILE:HG21	1.88	0.54
1:C:154:HIS:NE2	1:C:178:ALA:HB3	2.23	0.54
1:A:45:LEU:HB3	1:A:63:ILE:HD11	1.90	0.54
1:A:90:LEU:HA	1:A:93:LYS:HZ1	1.72	0.54
1:B:19:LEU:HD13	1:B:22:SER:CB	2.37	0.54
1:B:210:TRP:CD1	1:B:211:GLU:H	2.26	0.54
1:C:170:LEU:HD13	1:C:210:TRP:HB3	1.90	0.54
1:A:140:ILE:O	1:A:144:LEU:HG	2.07	0.54
1:D:27:PHE:HD2	1:D:74:SER:HG	1.56	0.54
1:A:30:ASP:CB	1:A:33:LYS:HB2	2.37	0.54
1:B:18:GLN:HB2	1:B:20:GLU:HB2	1.90	0.54
1:B:138:SER:HG	1:C:146:PHE:HE1	1.54	0.54
1:C:58:THR:HG23	1:C:92:ALA:HA	1.89	0.54
1:C:69:PHE:CE1	1:C:140:ILE:HA	2.43	0.54
1:A:131:GLN:HA	1:A:134:VAL:HG23	1.90	0.53
1:A:191:TYR:HB2	1:A:196:VAL:HG22	1.90	0.53
1:C:51:ARG:HD3	1:C:107:VAL:HG11	1.90	0.53
1:C:93:LYS:HA	1:C:98:PRO:CB	2.38	0.53
1:A:215:SER:HB2	1:A:217:ASP:OD1	2.08	0.53
1:B:74:SER:HB3	1:B:77:ARG:HG3	1.89	0.53
1:B:89:PHE:O	1:B:93:LYS:HD3	2.09	0.53
1:C:185:THR:HG21	1:C:187:PHE:CZ	2.44	0.53
1:D:120:ASP:HB3	1:D:123:SER:HB3	1.89	0.53
1:A:36:SER:O	1:A:40:GLN:HB2	2.08	0.53
1:B:252:LEU:HA	1:B:255:ILE:HD12	1.89	0.53
1:C:192:THR:CG2	1:C:194:PRO:HD2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ARG:HE	1:D:190:GLN:NE2	2.07	0.53
1:D:164:VAL:O	1:D:165:ARG:HB2	2.08	0.53
1:A:55:SER:OG	1:A:57:LEU:HD23	2.09	0.53
1:B:15:THR:OG1	1:B:17:GLU:HG3	2.07	0.53
1:B:68:ARG:HG3	1:B:189:LEU:HD21	1.89	0.53
1:B:199:VAL:HG12	1:B:241:PHE:HD1	1.73	0.53
1:C:30:ASP:OD1	1:C:31:PRO:HD2	2.07	0.53
1:A:48:MET:HG2	1:A:107:VAL:HG12	1.90	0.53
1:B:90:LEU:O	1:B:94:VAL:HG23	2.08	0.53
1:C:25:ARG:HD3	1:C:34:GLU:OE2	2.08	0.53
1:C:40:GLN:HA	1:C:43:ASN:OD1	2.09	0.53
1:C:194:PRO:HA	1:C:225:VAL:HG12	1.89	0.53
1:A:20:GLU:O	1:A:25:ARG:HG2	2.08	0.53
1:C:51:ARG:HH11	1:C:107:VAL:CG1	2.22	0.53
1:C:168:LYS:HG3	1:C:172:GLN:NE2	2.23	0.53
1:C:253:LYS:CA	1:C:256:TRP:HB2	2.36	0.53
1:D:82:SER:C	1:D:85:PRO:HD2	2.34	0.53
1:C:25:ARG:HB2	1:C:25:ARG:NH2	2.18	0.53
1:C:108:ALA:O	1:C:112:LEU:HB2	2.08	0.53
1:D:195:VAL:O	1:D:199:VAL:HG23	2.08	0.53
1:A:223:GLU:HA	1:A:226:ASP:O	2.09	0.53
1:C:20:GLU:HA	1:C:25:ARG:CZ	2.39	0.53
1:C:27:PHE:CE2	1:C:76:THR:HG21	2.44	0.53
1:D:84:ALA:O	1:D:88:LEU:HB2	2.09	0.53
1:A:44:LEU:O	1:A:84:ALA:HB1	2.09	0.53
1:A:68:ARG:HH12	1:A:150:ILE:HD11	1.74	0.53
1:C:51:ARG:NH1	1:C:107:VAL:HG13	2.23	0.53
1:C:222:TRP:HB2	1:C:229:VAL:CG1	2.39	0.53
1:C:160:CYS:O	1:C:164:VAL:HG22	2.09	0.52
1:A:226:ASP:OD1	1:A:229:VAL:HG23	2.09	0.52
1:D:140:ILE:HA	1:D:143:THR:HB	1.91	0.52
1:D:156:HIS:HB2	1:D:197:ALA:CB	2.39	0.52
1:A:231:LEU:HA	1:A:234:LEU:HB2	1.90	0.52
1:A:37:TYR:HD2	1:A:75:PHE:HB3	1.73	0.52
1:B:89:PHE:O	1:B:93:LYS:HG3	2.09	0.52
1:C:20:GLU:CA	1:C:25:ARG:HG2	2.38	0.52
1:C:51:ARG:NH1	1:C:107:VAL:HG22	2.24	0.52
1:A:12:TRP:O	1:A:189:LEU:HA	2.10	0.52
1:A:16:ARG:HG2	1:A:17:GLU:N	2.19	0.52
1:C:56:GLN:NE2	1:C:60:ASN:ND2	2.58	0.52
1:A:54:VAL:HG13	1:A:58:THR:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:SER:O	1:A:58:THR:HB	2.10	0.52
1:D:84:ALA:HB3	1:D:85:PRO:HD3	1.92	0.52
1:D:112:LEU:O	1:D:114:PRO:HD3	2.09	0.52
1:D:174:SER:HB3	1:D:201:ILE:HD13	1.90	0.52
1:A:45:LEU:HD22	1:A:63:ILE:HG12	1.92	0.52
1:A:164:VAL:O	1:A:165:ARG:HB2	2.10	0.52
1:A:203:LEU:HD12	1:A:238:THR:CA	2.40	0.52
1:B:29:VAL:HG11	1:B:37:TYR:HE2	1.75	0.52
1:B:39:GLN:HE21	1:B:184:LEU:CA	2.22	0.52
1:C:10:LYS:HD2	1:D:18:GLN:CD	2.35	0.52
1:D:16:ARG:CZ	1:D:190:GLN:HE21	2.22	0.52
1:D:55:SER:O	1:D:58:THR:HB	2.10	0.52
1:A:251:ARG:HE	1:A:254:ARG:HH21	1.55	0.52
1:B:84:ALA:HB3	1:B:85:PRO:HD3	1.92	0.52
1:C:230:THR:HG23	1:C:233:LEU:H	1.75	0.52
1:D:202:HIS:CD2	1:D:234:LEU:HB3	2.45	0.52
1:B:112:LEU:O	1:B:114:PRO:HD3	2.09	0.51
1:C:130:VAL:O	1:C:130:VAL:HG12	2.11	0.51
1:D:64:VAL:HG11	1:D:150:ILE:CG2	2.40	0.51
1:B:242:LEU:O	1:B:246:GLU:HB2	2.11	0.51
1:A:219:LYS:HD2	1:A:223:GLU:OE1	2.10	0.51
1:B:177:MET:HB3	1:B:200:CYS:HB3	1.92	0.51
1:C:136:LEU:HD23	1:C:136:LEU:N	2.25	0.51
1:A:125:ALA:O	1:A:129:GLN:OE1	2.29	0.51
1:B:174:SER:HB3	1:B:201:ILE:HD13	1.91	0.51
1:C:57:LEU:O	1:C:61:THR:OG1	2.28	0.51
1:C:78:PHE:CZ	1:C:139:ILE:HG21	2.44	0.51
1:D:68:ARG:HG3	1:D:189:LEU:HD21	1.93	0.51
1:D:96:GLU:O	1:D:96:GLU:HG3	2.09	0.51
1:D:259:ARG:HA	1:D:262:GLU:HB3	1.91	0.51
1:A:228:THR:CG2	1:B:21:ASN:HB2	2.41	0.51
1:C:105:ILE:HD11	1:C:133:LEU:CD1	2.41	0.51
1:C:221:TRP:HA	1:C:224:TYR:HE1	1.74	0.51
1:D:13:TYR:HA	1:D:189:LEU:O	2.10	0.51
1:D:38:ARG:HG3	1:D:75:PHE:CZ	2.45	0.51
1:D:190:GLN:HB3	1:D:191:TYR:CD2	2.46	0.51
1:A:84:ALA:HB3	1:A:85:PRO:HD3	1.93	0.51
1:B:69:PHE:HE1	1:B:139:ILE:HG22	1.76	0.51
1:C:20:GLU:OE1	1:D:228:THR:HB	2.10	0.51
1:C:141:LEU:HD22	1:C:146:PHE:HA	1.93	0.51
1:A:142:GLN:OE1	1:D:141:LEU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HA	1:B:26:ARG:HH11	1.75	0.51
1:C:56:GLN:HG3	1:C:60:ASN:ND2	2.23	0.51
1:C:202:HIS:ND1	1:C:206:LYS:HB2	2.26	0.51
1:A:156:HIS:HA	1:A:159:LYS:HD2	1.91	0.51
1:C:132:ASP:O	1:C:136:LEU:HG	2.10	0.51
1:C:185:THR:HG23	1:C:244:ILE:HD11	1.92	0.51
1:C:222:TRP:CD1	1:C:229:VAL:HG12	2.46	0.51
1:C:178:ALA:HA	1:C:200:CYS:SG	2.50	0.50
1:D:192:THR:OG1	1:D:195:VAL:HG23	2.11	0.50
1:A:25:ARG:HH22	1:A:31:PRO:HA	1.77	0.50
1:A:45:LEU:HB3	1:A:63:ILE:CD1	2.41	0.50
1:A:89:PHE:HE1	1:A:99:LYS:O	1.95	0.50
1:C:16:ARG:HD2	1:D:233:LEU:CD1	2.39	0.50
1:D:16:ARG:NE	1:D:190:GLN:HE21	2.09	0.50
1:A:44:LEU:HD21	1:A:81:ASN:O	2.11	0.50
1:A:145:GLY:CA	1:D:142:GLN:HE22	2.24	0.50
1:B:21:ASN:OD1	1:B:21:ASN:O	2.30	0.50
1:B:23:PRO:HG2	1:B:72:ILE:HA	1.92	0.50
1:B:124:GLU:OE1	1:B:127:LEU:HB2	2.11	0.50
1:D:93:LYS:CA	1:D:98:PRO:HB3	2.41	0.50
1:D:203:LEU:HD13	1:D:241:PHE:CD1	2.46	0.50
1:A:93:LYS:CG	1:A:98:PRO:HB3	2.41	0.50
1:B:128:GLN:O	1:B:131:GLN:OE1	2.30	0.50
1:C:150:ILE:HG23	1:C:150:ILE:O	2.11	0.50
1:C:161:THR:O	1:C:164:VAL:HG22	2.11	0.50
1:D:60:ASN:O	1:D:64:VAL:HG23	2.12	0.50
1:B:253:LYS:O	1:B:257:ASN:OD1	2.30	0.50
1:C:42:ALA:HA	1:C:45:LEU:HD12	1.91	0.50
1:C:56:GLN:CG	1:C:60:ASN:HD21	2.23	0.50
1:C:62:ALA:HB1	1:C:88:LEU:HG	1.93	0.50
1:D:93:LYS:O	1:D:95:GLU:O	2.29	0.50
1:D:204:ALA:O	1:D:208:SER:OG	2.29	0.50
1:A:231:LEU:O	1:A:235:ASP:OD1	2.30	0.50
1:C:44:LEU:O	1:C:48:MET:N	2.42	0.50
1:C:83:VAL:O	1:C:86:ALA:HB3	2.12	0.50
1:C:89:PHE:O	1:C:93:LYS:HG2	2.12	0.50
1:A:94:VAL:HG22	1:A:148:LEU:HG	1.93	0.50
1:A:214:VAL:HG13	1:A:221:TRP:HB3	1.93	0.50
1:C:54:VAL:CG1	1:C:59:ILE:HG13	2.41	0.50
1:C:92:ALA:O	1:C:98:PRO:HA	2.12	0.50
1:C:226:ASP:CB	1:C:229:VAL:HG23	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLU:OE1	1:D:228:THR:HA	2.11	0.50
1:C:89:PHE:CE2	1:C:101:LEU:HD23	2.47	0.50
1:D:155:THR:O	1:D:159:LYS:HG3	2.12	0.50
1:A:45:LEU:HD23	1:A:59:ILE:HG23	1.94	0.50
1:A:69:PHE:CD1	1:A:140:ILE:HG13	2.47	0.50
1:C:79:PRO:O	1:C:83:VAL:HG23	2.12	0.50
1:B:12:TRP:CZ2	1:B:144:LEU:HA	2.47	0.49
1:C:51:ARG:HH12	1:C:110:THR:HB	1.76	0.49
1:C:204:ALA:O	1:C:208:SER:OG	2.30	0.49
1:B:190:GLN:HB3	1:B:191:TYR:CE2	2.48	0.49
1:D:102:GLU:HB2	1:D:126:TYR:OH	2.12	0.49
1:B:40:GLN:HA	2:B:363:HOH:O	2.11	0.49
1:C:71:MET:HG3	1:C:189:LEU:HD22	1.92	0.49
1:C:177:MET:HG2	1:C:203:LEU:CB	2.42	0.49
1:C:68:ARG:CB	1:C:189:LEU:HD11	2.42	0.49
1:D:30:ASP:OD1	1:D:31:PRO:HD2	2.12	0.49
1:D:140:ILE:HG12	1:D:144:LEU:CD1	2.38	0.49
1:D:241:PHE:CD2	1:D:245:LEU:HD11	2.47	0.49
1:A:90:LEU:O	1:A:94:VAL:HG23	2.12	0.49
1:C:70:TYR:OH	1:C:80:GLY:HA2	2.11	0.49
1:D:123:SER:O	1:D:127:LEU:HG	2.13	0.49
1:B:67:HIS:O	1:B:71:MET:HG2	2.12	0.49
1:D:92:ALA:O	1:D:95:GLU:O	2.30	0.49
1:C:92:ALA:O	1:C:97:GLN:O	2.30	0.49
1:D:89:PHE:HE1	1:D:99:LYS:O	1.96	0.49
1:D:222:TRP:O	1:D:226:ASP:O	2.30	0.49
1:B:77:ARG:HH21	1:B:78:PHE:HZ	1.59	0.49
1:D:22:SER:HB2	1:D:25:ARG:NH2	2.27	0.49
1:A:90:LEU:CG	1:A:141:LEU:HG	2.43	0.49
1:B:27:PHE:HE2	1:B:74:SER:HB2	1.77	0.49
1:C:118:LEU:HD22	1:C:119:PRO:CD	2.42	0.49
1:D:16:ARG:O	1:D:20:GLU:OE2	2.30	0.49
1:D:195:VAL:O	1:D:195:VAL:HG12	2.13	0.49
1:B:70:TYR:OH	1:B:83:VAL:HG21	2.12	0.49
1:B:233:LEU:CA	1:B:236:GLU:HB3	2.37	0.49
1:C:126:TYR:O	1:C:130:VAL:HG23	2.13	0.49
1:B:52:LEU:CD2	1:B:99:LYS:HG3	2.40	0.48
1:B:172:GLN:O	1:B:176:PHE:HB2	2.13	0.48
1:C:62:ALA:CB	1:C:88:LEU:HG	2.43	0.48
1:D:194:PRO:HB2	1:D:226:ASP:OD2	2.13	0.48
1:D:222:TRP:O	1:D:229:VAL:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLN:HG3	1:A:50:GLN:OE1	2.12	0.48
1:C:82:SER:O	1:C:85:PRO:HG2	2.13	0.48
1:B:132:ASP:O	1:B:136:LEU:HB2	2.13	0.48
1:B:160:CYS:O	1:B:164:VAL:HG22	2.13	0.48
1:B:101:LEU:HD21	1:B:133:LEU:HD12	1.96	0.48
1:D:47:ASP:HA	1:D:50:GLN:HE21	1.78	0.48
1:A:93:LYS:HG2	1:A:98:PRO:HB3	1.95	0.48
1:B:173:THR:O	1:B:177:MET:HB2	2.14	0.48
1:C:221:TRP:HA	1:C:224:TYR:CE1	2.48	0.48
1:C:239:HIS:HA	1:C:242:LEU:CD1	2.32	0.48
1:A:94:VAL:HG22	1:A:148:LEU:CG	2.44	0.48
1:B:223:GLU:HA	1:B:226:ASP:O	2.14	0.48
1:B:253:LYS:HA	1:B:256:TRP:HB2	1.96	0.48
1:C:156:HIS:CB	1:C:225:VAL:HG13	2.44	0.48
1:C:158:VAL:HG12	1:C:158:VAL:O	2.13	0.48
1:B:127:LEU:HA	1:B:130:VAL:CG2	2.43	0.48
1:C:122:ARG:HG3	1:C:123:SER:N	2.29	0.48
1:C:222:TRP:HD1	1:C:229:VAL:O	1.97	0.48
1:C:252:LEU:HA	1:C:255:ILE:CD1	2.44	0.48
1:A:19:LEU:O	1:A:22:SER:OG	2.30	0.48
1:A:195:VAL:HG12	1:A:195:VAL:O	2.13	0.48
1:B:83:VAL:O	1:B:86:ALA:HB3	2.14	0.48
1:B:259:ARG:HA	1:B:262:GLU:CG	2.31	0.48
1:C:241:PHE:CE2	1:C:245:LEU:HD21	2.49	0.48
1:D:29:VAL:CG1	1:D:33:LYS:HB3	2.35	0.48
1:A:23:PRO:HA	1:A:26:ARG:HG3	1.95	0.48
1:A:128:GLN:O	1:A:131:GLN:OE1	2.32	0.48
1:B:211:GLU:O	1:B:213:PRO:HD3	2.13	0.48
1:C:93:LYS:HG3	1:C:94:VAL:N	2.28	0.48
1:C:196:VAL:HG12	1:C:196:VAL:O	2.14	0.48
1:A:192:THR:O	1:A:196:VAL:HG23	2.14	0.48
1:B:195:VAL:HG12	1:B:195:VAL:O	2.14	0.48
1:B:46:GLN:NE2	1:B:59:ILE:HG21	2.29	0.47
1:B:68:ARG:O	1:B:71:MET:HB2	2.14	0.47
1:C:35:LEU:O	1:C:39:GLN:OE1	2.32	0.47
1:D:207:TRP:CH2	1:D:255:ILE:HG22	2.47	0.47
1:A:120:ASP:HB3	1:A:123:SER:HB3	1.96	0.47
1:B:16:ARG:HG3	1:B:18:GLN:HG2	1.96	0.47
1:D:38:ARG:HG3	1:D:75:PHE:HZ	1.79	0.47
1:A:12:TRP:HB3	1:A:68:ARG:CZ	2.44	0.47
1:C:107:VAL:HG13	1:C:111:CYS:SG	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LEU:HD12	1:C:241:PHE:CE1	2.49	0.47
1:D:23:PRO:HA	1:D:26:ARG:CD	2.44	0.47
1:D:39:GLN:HG2	1:D:184:LEU:O	2.14	0.47
1:C:93:LYS:HA	1:C:98:PRO:HA	1.96	0.47
1:A:58:THR:HG23	1:A:95:GLU:CG	2.45	0.47
1:A:145:GLY:HA2	1:D:142:GLN:CD	2.39	0.47
1:A:164:VAL:HB	1:A:212:ILE:CG2	2.44	0.47
1:B:12:TRP:HA	1:B:14:PHE:CE1	2.50	0.47
1:C:162:GLN:H	1:C:162:GLN:CD	2.23	0.47
1:A:48:MET:O	1:A:51:ARG:HB2	2.13	0.47
1:B:253:LYS:HG2	1:B:257:ASN:OD1	2.14	0.47
1:C:41:ALA:HA	1:C:44:LEU:CD2	2.45	0.47
1:A:90:LEU:CD1	1:A:141:LEU:HG	2.45	0.47
1:A:201:ILE:O	1:A:205:CYS:HB2	2.14	0.47
1:A:251:ARG:HD3	1:A:254:ARG:NE	2.26	0.47
1:B:252:LEU:HD11	1:B:256:TRP:NE1	2.29	0.47
1:C:16:ARG:HA	1:C:19:LEU:CB	2.39	0.47
1:C:42:ALA:HA	1:C:45:LEU:HD13	1.96	0.47
1:C:51:ARG:HH11	1:C:107:VAL:HG22	1.79	0.47
1:C:120:ASP:OD2	1:C:121:THR:N	2.48	0.47
1:C:138:SER:O	1:C:142:GLN:NE2	2.47	0.47
1:C:141:LEU:HD23	1:C:141:LEU:HA	1.76	0.47
1:D:208:SER:O	1:D:209:ASN:HB2	2.14	0.47
1:A:45:LEU:CD2	1:A:59:ILE:HG23	2.44	0.47
1:A:82:SER:C	1:A:85:PRO:HD2	2.39	0.47
1:A:230:THR:O	1:A:234:LEU:HB2	2.15	0.47
1:B:214:VAL:CG1	1:B:221:TRP:HB3	2.45	0.47
1:C:90:LEU:HD12	1:C:94:VAL:HG23	1.96	0.47
1:C:154:HIS:O	1:C:157:VAL:N	2.48	0.47
1:A:152:HIS:HB3	1:A:154:HIS:ND1	2.29	0.47
1:B:42:ALA:HB1	1:B:63:ILE:HD12	1.96	0.47
1:B:138:SER:OG	1:C:146:PHE:HE1	1.98	0.47
1:A:64:VAL:O	1:A:68:ARG:HG3	2.14	0.47
1:A:83:VAL:O	1:A:86:ALA:HB3	2.15	0.47
1:A:101:LEU:O	1:A:101:LEU:HD22	2.15	0.47
1:B:66:MET:HG2	1:B:70:TYR:CE2	2.50	0.47
1:B:214:VAL:HG13	1:B:221:TRP:HB3	1.97	0.47
1:C:125:ALA:O	1:C:126:TYR:HB3	2.13	0.47
1:D:94:VAL:CG2	1:D:148:LEU:HD23	2.45	0.47
1:D:214:VAL:HG12	1:D:215:SER:H	1.79	0.47
1:B:18:GLN:HB2	1:B:20:GLU:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ARG:O	1:C:25:ARG:HG3	2.14	0.46
1:C:247:LYS:HE3	1:C:247:LYS:HA	1.97	0.46
1:C:54:VAL:O	1:C:54:VAL:HG12	2.14	0.46
1:C:56:GLN:NE2	1:C:59:ILE:HB	2.29	0.46
1:C:147:GLU:O	1:C:148:LEU:HG	2.15	0.46
1:C:198:CYS:HB3	1:C:234:LEU:CD2	2.46	0.46
1:B:168:LYS:CD	1:B:172:GLN:HE22	2.29	0.46
1:D:11:ARG:HG3	1:D:11:ARG:HH11	1.79	0.46
1:D:178:ALA:HA	1:D:200:CYS:SG	2.56	0.46
1:D:251:ARG:NH1	1:D:254:ARG:HB3	2.27	0.46
1:C:50:GLN:HG3	1:C:59:ILE:CD1	2.34	0.46
1:C:135:ILE:HG22	1:C:136:LEU:HD23	1.97	0.46
1:C:248:THR:O	1:C:252:LEU:HB3	2.15	0.46
1:D:16:ARG:HE	1:D:190:GLN:HE21	1.62	0.46
1:C:46:GLN:O	1:C:50:GLN:OE1	2.34	0.46
1:A:93:LYS:HB2	1:A:93:LYS:HE2	1.39	0.46
1:A:230:THR:O	1:A:234:LEU:HD22	2.15	0.46
1:B:138:SER:HB2	1:C:138:SER:OG	2.15	0.46
1:B:153:PRO:HD2	1:B:154:HIS:CE1	2.51	0.46
1:C:16:ARG:CA	1:C:19:LEU:HD12	2.46	0.46
1:C:89:PHE:HD1	1:C:89:PHE:HA	1.64	0.46
1:A:71:MET:HE2	1:A:71:MET:HB3	1.79	0.46
1:A:142:GLN:O	1:D:142:GLN:NE2	2.49	0.46
1:B:155:THR:O	1:B:158:VAL:HG23	2.16	0.46
1:B:157:VAL:O	1:B:161:THR:OG1	2.30	0.46
1:B:219:LYS:HB3	1:B:219:LYS:HE3	1.53	0.46
1:C:252:LEU:HA	1:C:255:ILE:HD12	1.97	0.46
1:D:226:ASP:HB3	1:D:229:VAL:CG2	2.42	0.46
1:A:131:GLN:C	1:A:134:VAL:HG23	2.40	0.46
1:B:153:PRO:HB3	1:B:196:VAL:HB	1.98	0.46
1:C:20:GLU:O	1:C:25:ARG:HG2	2.16	0.46
1:C:207:TRP:CZ3	1:C:259:ARG:HG3	2.51	0.46
1:D:92:ALA:HB1	1:D:98:PRO:CA	2.39	0.46
1:A:14:PHE:CE1	1:A:71:MET:HE2	2.51	0.45
1:B:46:GLN:NE2	1:B:183:HIS:HE1	2.14	0.45
1:B:59:ILE:O	1:B:62:ALA:HB3	2.16	0.45
1:B:103:HIS:O	1:B:107:VAL:HG23	2.15	0.45
1:B:155:THR:O	1:B:159:LYS:HE2	2.16	0.45
1:C:127:LEU:O	1:C:131:GLN:N	2.49	0.45
1:C:128:GLN:HA	1:C:131:GLN:CB	2.42	0.45
1:C:140:ILE:HG13	1:C:144:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:LYS:HA	1:D:33:LYS:HD2	1.53	0.45
1:A:16:ARG:HH11	1:B:233:LEU:HD11	1.81	0.45
1:C:20:GLU:OE2	1:C:25:ARG:HG3	2.17	0.45
1:D:68:ARG:HG3	1:D:189:LEU:CD2	2.46	0.45
1:D:151:ASP:HB2	1:D:193:PRO:HG2	1.98	0.45
1:A:45:LEU:HD22	1:A:63:ILE:CD1	2.46	0.45
1:A:62:ALA:O	1:A:65:TYR:HB2	2.16	0.45
1:A:259:ARG:HG2	1:A:259:ARG:O	2.16	0.45
1:B:23:PRO:HG2	1:B:72:ILE:C	2.41	0.45
1:D:236:GLU:O	1:D:240:GLU:HB2	2.16	0.45
1:A:109:HIS:O	1:A:113:HIS:N	2.50	0.45
1:A:153:PRO:CA	1:A:197:ALA:HB2	2.47	0.45
1:B:47:ASP:OD1	1:B:50:GLN:NE2	2.50	0.45
1:B:131:GLN:O	1:B:135:ILE:N	2.50	0.45
1:B:151:ASP:OD2	1:B:151:ASP:N	2.50	0.45
1:C:19:LEU:O	1:C:25:ARG:NH2	2.50	0.45
1:D:47:ASP:OD1	1:D:50:GLN:NE2	2.49	0.45
1:A:97:GLN:O	1:A:97:GLN:NE2	2.50	0.45
1:A:235:ASP:OD1	1:A:235:ASP:N	2.50	0.45
1:A:243:GLN:O	1:A:247:LYS:NZ	2.50	0.45
1:B:39:GLN:NE2	1:B:184:LEU:O	2.50	0.45
1:B:217:ASP:OD1	1:B:218:GLY:N	2.50	0.45
1:B:247:LYS:HD3	1:B:247:LYS:HA	1.48	0.45
1:C:22:SER:O	1:C:25:ARG:N	2.50	0.45
1:C:118:LEU:HD22	1:C:118:LEU:HA	1.85	0.45
1:C:238:THR:O	1:C:241:PHE:HB3	2.16	0.45
1:D:8:ASN:ND2	1:D:151:ASP:OD2	2.50	0.45
1:D:125:ALA:O	1:D:129:GLN:NE2	2.50	0.45
1:A:195:VAL:HB	1:B:16:ARG:HH22	1.81	0.45
1:C:84:ALA:HB1	1:C:88:LEU:CD1	2.46	0.45
1:C:89:PHE:O	1:C:93:LYS:HB3	2.16	0.45
1:D:47:ASP:HA	1:D:50:GLN:NE2	2.32	0.45
1:D:137:GLU:O	1:D:137:GLU:HG2	2.13	0.45
1:A:22:SER:H	1:A:25:ARG:HE	1.64	0.45
1:B:44:LEU:CD2	1:B:81:ASN:HA	2.47	0.45
1:B:53:ASN:ND2	2:B:368:HOH:O	2.50	0.45
1:B:102:GLU:O	1:B:106:LYS:N	2.50	0.45
1:C:39:GLN:O	1:C:42:ALA:N	2.50	0.45
1:C:254:ARG:O	1:C:258:TRP:N	2.49	0.45
1:D:46:GLN:CD	1:D:56:GLN:HE22	2.24	0.45
1:A:150:ILE:O	1:A:150:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG11	1:A:221:TRP:N	2.31	0.45
1:C:39:GLN:HG2	1:C:183:HIS:O	2.17	0.45
1:C:84:ALA:N	1:C:85:PRO:HD2	2.32	0.45
1:D:46:GLN:NE2	1:D:56:GLN:OE1	2.50	0.45
1:D:180:ASN:OD1	1:D:255:ILE:HD11	2.17	0.45
1:A:131:GLN:O	1:A:134:VAL:HG23	2.17	0.45
1:B:55:SER:O	1:B:58:THR:HB	2.16	0.45
1:C:169:ASP:OD2	1:C:262:GLU:HB2	2.16	0.45
1:D:16:ARG:O	1:D:19:LEU:N	2.50	0.45
1:D:173:THR:O	1:D:177:MET:HB2	2.17	0.45
1:A:252:LEU:HD11	1:A:256:TRP:NE1	2.32	0.45
1:B:15:THR:N	1:B:17:GLU:OE2	2.50	0.45
1:B:127:LEU:HD21	2:B:364:HOH:O	2.16	0.45
1:C:79:PRO:O	1:C:83:VAL:N	2.50	0.45
1:D:16:ARG:HH21	1:D:190:GLN:NE2	2.08	0.45
1:D:84:ALA:O	1:D:88:LEU:N	2.49	0.45
1:D:150:ILE:HG22	1:D:150:ILE:O	2.17	0.45
1:D:207:TRP:C	1:D:259:ARG:HH22	2.25	0.45
1:D:241:PHE:O	1:D:245:LEU:HD12	2.17	0.45
1:A:8:ASN:N	2:A:360:HOH:O	2.50	0.44
1:A:214:VAL:CG1	1:A:215:SER:H	2.27	0.44
1:B:21:ASN:OD1	1:B:26:ARG:NH2	2.50	0.44
1:B:138:SER:CA	1:B:141:LEU:HB2	2.34	0.44
1:B:146:PHE:CE2	1:C:142:GLN:HG3	2.52	0.44
1:B:184:LEU:HD11	1:B:251:ARG:HB3	2.00	0.44
1:C:173:THR:HG22	1:C:173:THR:O	2.16	0.44
1:A:251:ARG:HD3	1:A:251:ARG:HA	1.75	0.44
1:A:252:LEU:O	1:A:255:ILE:N	2.49	0.44
1:B:97:GLN:O	1:B:97:GLN:NE2	2.50	0.44
1:B:243:GLN:HA	1:B:246:GLU:CB	2.46	0.44
1:C:89:PHE:CZ	1:C:101:LEU:HD23	2.53	0.44
1:D:94:VAL:HG22	1:D:148:LEU:HD23	1.98	0.44
1:D:159:LYS:HG3	1:D:159:LYS:H	1.39	0.44
1:A:154:HIS:HA	1:A:157:VAL:HB	1.99	0.44
1:B:109:HIS:NE2	1:B:117:SER:O	2.50	0.44
1:B:136:LEU:HD23	1:B:139:ILE:HB	1.99	0.44
1:C:52:LEU:HD11	1:C:104:VAL:HG13	1.99	0.44
1:C:156:HIS:CG	1:C:225:VAL:HG13	2.52	0.44
1:C:162:GLN:O	1:C:165:ARG:N	2.50	0.44
1:C:254:ARG:O	1:C:258:TRP:HB2	2.17	0.44
1:D:42:ALA:CB	1:D:63:ILE:HD12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:TRP:CD1	1:D:211:GLU:H	2.35	0.44
1:A:67:HIS:NE2	1:A:182:LEU:O	2.50	0.44
1:A:148:LEU:HD12	1:A:148:LEU:N	2.32	0.44
1:B:130:VAL:HG12	1:B:131:GLN:N	2.33	0.44
1:B:208:SER:O	1:B:209:ASN:HB2	2.15	0.44
1:B:242:LEU:O	1:B:246:GLU:N	2.50	0.44
1:C:39:GLN:O	1:C:43:ASN:N	2.51	0.44
1:C:44:LEU:N	1:C:44:LEU:HD13	2.32	0.44
1:C:70:TYR:HE1	1:C:74:SER:O	2.00	0.44
1:C:84:ALA:O	1:C:88:LEU:HD12	2.17	0.44
1:C:215:SER:N	1:C:219:LYS:O	2.50	0.44
1:D:30:ASP:CB	1:D:33:LYS:HB2	2.48	0.44
1:A:62:ALA:O	1:A:65:TYR:N	2.50	0.44
1:B:21:ASN:HD21	1:B:26:ARG:NH2	2.13	0.44
1:C:207:TRP:CH2	1:C:259:ARG:HG3	2.53	0.44
1:D:14:PHE:CD1	1:D:71:MET:HE2	2.53	0.44
1:A:146:PHE:CZ	1:D:139:ILE:HA	2.48	0.44
1:A:159:LYS:HB2	1:A:163:LEU:CD1	2.48	0.44
1:B:46:GLN:HB2	1:B:183:HIS:CE1	2.52	0.44
1:C:156:HIS:O	1:C:160:CYS:N	2.49	0.44
1:C:237:LEU:HD23	1:C:237:LEU:HA	1.80	0.44
1:D:20:GLU:O	1:D:25:ARG:NE	2.50	0.44
1:D:59:ILE:O	1:D:62:ALA:HB3	2.17	0.44
1:A:156:HIS:HA	1:A:159:LYS:NZ	2.33	0.44
1:B:90:LEU:HD21	1:B:141:LEU:HA	2.00	0.44
1:B:148:LEU:N	1:B:148:LEU:HD12	2.33	0.44
1:C:39:GLN:O	1:C:43:ASN:ND2	2.50	0.44
1:C:65:TYR:O	1:C:87:ALA:HB2	2.17	0.44
1:A:33:LYS:O	1:A:36:SER:N	2.50	0.44
1:A:52:LEU:HD21	1:A:107:VAL:HG21	2.00	0.44
1:A:131:GLN:O	1:A:135:ILE:N	2.50	0.44
1:B:101:LEU:O	1:B:101:LEU:HD22	2.18	0.44
1:D:177:MET:HE2	1:D:203:LEU:CD2	2.37	0.44
1:D:222:TRP:HB2	1:D:229:VAL:CG1	2.48	0.44
1:A:22:SER:H	1:A:25:ARG:NE	2.15	0.44
1:A:85:PRO:CB	1:A:133:LEU:HD11	2.47	0.44
1:B:133:LEU:HD22	1:B:133:LEU:HA	1.89	0.44
1:B:179:THR:O	1:B:179:THR:HG22	2.18	0.44
1:D:93:LYS:HA	1:D:98:PRO:HB3	1.98	0.44
1:B:168:LYS:CE	1:B:172:GLN:HE22	2.31	0.43
1:C:164:VAL:O	1:C:165:ARG:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:MET:HE3	1:D:66:MET:HB3	1.82	0.43
1:C:241:PHE:O	1:C:245:LEU:HD12	2.19	0.43
1:A:32:ASP:O	1:A:36:SER:N	2.51	0.43
1:B:19:LEU:HD12	1:B:34:GLU:CD	2.44	0.43
1:B:23:PRO:HG2	1:B:72:ILE:CA	2.48	0.43
1:B:125:ALA:O	1:B:129:GLN:OE1	2.35	0.43
1:C:35:LEU:HD13	1:C:35:LEU:HA	1.79	0.43
1:C:42:ALA:HB2	1:C:66:MET:CE	2.48	0.43
1:C:94:VAL:HG12	1:C:95:GLU:N	2.33	0.43
1:C:207:TRP:CH2	1:C:255:ILE:HG22	2.48	0.43
1:D:71:MET:HE2	1:D:71:MET:HB3	1.92	0.43
1:D:133:LEU:HD22	1:D:133:LEU:HA	1.83	0.43
1:D:262:GLU:O	1:D:263:ALA:HB2	2.18	0.43
1:A:90:LEU:HD22	1:A:140:ILE:HG23	2.00	0.43
1:B:19:LEU:N	1:B:19:LEU:HD23	2.32	0.43
1:B:94:VAL:HG22	1:B:148:LEU:HD23	2.01	0.43
1:C:198:CYS:SG	1:C:229:VAL:HG11	2.58	0.43
1:D:77:ARG:H	1:D:77:ARG:HG3	1.67	0.43
1:D:77:ARG:O	1:D:79:PRO:HD3	2.19	0.43
1:D:131:GLN:O	1:D:135:ILE:HB	2.18	0.43
1:D:142:GLN:O	1:D:142:GLN:HG3	2.18	0.43
1:D:230:THR:O	1:D:234:LEU:HD22	2.18	0.43
1:A:208:SER:O	1:A:209:ASN:HB2	2.19	0.43
1:A:226:ASP:HB3	1:A:229:VAL:HG23	1.99	0.43
1:B:203:LEU:HD12	1:B:238:THR:HA	2.00	0.43
1:C:198:CYS:SG	1:C:222:TRP:HA	2.58	0.43
1:A:16:ARG:HB2	2:A:377:HOH:O	2.18	0.43
1:B:48:MET:O	1:B:51:ARG:HB2	2.19	0.43
1:B:185:THR:HG22	1:B:244:ILE:CG2	2.48	0.43
1:D:24:SER:OG	1:D:34:GLU:OE1	2.30	0.43
1:A:20:GLU:OE1	1:A:31:PRO:HB3	2.18	0.43
1:A:46:GLN:HA	1:A:59:ILE:HG21	2.00	0.43
1:A:137:GLU:HG3	1:A:137:GLU:O	2.18	0.43
1:B:150:ILE:O	1:B:150:ILE:HG22	2.17	0.43
1:C:170:LEU:HD21	1:C:205:CYS:SG	2.59	0.43
1:C:244:ILE:HG22	1:C:248:THR:HG21	2.01	0.43
1:D:14:PHE:HB2	1:D:19:LEU:HD23	2.00	0.43
1:D:30:ASP:HB2	1:D:33:LYS:HB2	2.01	0.43
1:D:69:PHE:CE2	1:D:73:GLN:HG3	2.54	0.43
1:A:130:VAL:HG12	1:A:131:GLN:N	2.34	0.43
1:A:179:THR:HG23	1:A:183:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:PHE:HB3	1:B:17:GLU:OE2	2.18	0.43
1:B:226:ASP:OD1	1:B:228:THR:HG23	2.19	0.43
1:C:93:LYS:HA	1:C:98:PRO:CA	2.48	0.43
1:C:194:PRO:O	1:C:197:ALA:HB3	2.19	0.43
1:D:53:ASN:HD22	1:D:53:ASN:HA	1.62	0.43
1:D:130:VAL:HG12	1:D:131:GLN:N	2.33	0.43
1:A:184:LEU:HD23	1:A:184:LEU:N	2.33	0.43
1:A:199:VAL:O	1:A:203:LEU:HB2	2.19	0.43
1:A:199:VAL:HG12	1:A:241:PHE:HD1	1.84	0.43
1:A:236:GLU:O	1:A:240:GLU:HB2	2.19	0.43
1:B:248:THR:O	1:B:252:LEU:HB3	2.18	0.43
1:C:133:LEU:CA	1:C:136:LEU:HG	2.47	0.43
1:C:230:THR:CG2	1:C:233:LEU:H	2.32	0.43
1:D:148:LEU:HD12	1:D:148:LEU:N	2.34	0.43
1:A:53:ASN:HD22	1:A:53:ASN:HA	1.62	0.42
1:A:186:THR:HB	1:A:189:LEU:HD12	2.01	0.42
1:B:226:ASP:HB3	1:B:229:VAL:CG2	2.42	0.42
1:C:199:VAL:HA	1:C:234:LEU:HD11	2.00	0.42
1:D:34:GLU:HG3	1:D:75:PHE:CE2	2.54	0.42
1:A:140:ILE:HG12	1:A:144:LEU:CD1	2.37	0.42
1:B:32:ASP:O	1:B:35:LEU:HD23	2.19	0.42
1:B:39:GLN:HE21	1:B:184:LEU:C	2.27	0.42
1:D:156:HIS:CE1	1:D:194:PRO:HB3	2.54	0.42
1:A:10:LYS:O	1:A:12:TRP:NE1	2.52	0.42
1:A:251:ARG:O	1:A:255:ILE:HG13	2.19	0.42
1:B:18:GLN:HB2	1:B:20:GLU:HG3	2.01	0.42
1:C:208:SER:O	1:C:209:ASN:HB3	2.19	0.42
1:C:226:ASP:HB3	1:C:229:VAL:HG23	2.00	0.42
1:D:101:LEU:HD22	1:D:101:LEU:O	2.19	0.42
1:A:154:HIS:O	1:A:157:VAL:HB	2.20	0.42
1:A:180:ASN:OD1	1:A:184:LEU:HG	2.20	0.42
1:A:219:LYS:HB3	1:A:219:LYS:HE3	1.52	0.42
1:A:241:PHE:O	1:A:245:LEU:HD12	2.20	0.42
1:B:66:MET:O	1:B:70:TYR:HD2	2.03	0.42
1:B:134:VAL:HA	1:B:137:GLU:HB3	2.01	0.42
1:C:24:SER:O	1:C:29:VAL:HB	2.20	0.42
1:C:45:LEU:CD2	1:C:88:LEU:HD11	2.48	0.42
1:C:132:ASP:O	1:C:136:LEU:CG	2.67	0.42
1:C:251:ARG:NH2	2:C:377:HOH:O	2.49	0.42
1:D:14:PHE:HB2	1:D:19:LEU:CD2	2.50	0.42
1:B:46:GLN:HE21	1:B:183:HIS:HE1	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:MET:HE2	1:B:88:LEU:HD23	2.02	0.42
1:B:64:VAL:HG22	1:B:182:LEU:HD21	2.01	0.42
1:C:83:VAL:O	1:C:86:ALA:N	2.50	0.42
1:D:97:GLN:HE21	1:D:97:GLN:HB3	1.58	0.42
1:D:214:VAL:HG21	1:D:221:TRP:CB	2.34	0.42
1:A:38:ARG:O	1:A:42:ALA:N	2.50	0.42
1:D:184:LEU:N	1:D:184:LEU:HD23	2.33	0.42
1:B:93:LYS:N	1:B:98:PRO:HB3	2.35	0.42
1:B:184:LEU:N	1:B:184:LEU:HD23	2.34	0.42
1:C:78:PHE:HA	1:C:79:PRO:HD3	1.87	0.42
1:D:214:VAL:CG2	1:D:221:TRP:HB3	2.34	0.42
1:A:105:ILE:HD11	1:A:133:LEU:CB	2.50	0.42
1:B:102:GLU:HG2	1:B:106:LYS:HD2	2.02	0.42
1:C:168:LYS:O	1:C:172:GLN:HB2	2.19	0.42
1:C:251:ARG:NH1	1:C:254:ARG:HH12	2.17	0.42
1:D:14:PHE:N	1:D:189:LEU:O	2.50	0.42
1:A:62:ALA:HB2	1:A:91:ALA:CB	2.50	0.42
1:A:244:ILE:O	1:A:244:ILE:HG22	2.20	0.42
1:C:54:VAL:HG22	1:C:58:THR:CG2	2.49	0.42
1:D:101:LEU:CD2	1:D:133:LEU:HD12	2.50	0.42
1:A:102:GLU:O	1:A:106:LYS:N	2.53	0.42
1:A:131:GLN:CA	1:A:134:VAL:HG23	2.48	0.42
1:B:245:LEU:O	1:B:252:LEU:HD13	2.20	0.42
1:C:20:GLU:HG2	1:C:25:ARG:HG2	2.02	0.42
1:B:25:ARG:HD3	1:B:25:ARG:HA	1.75	0.41
1:B:45:LEU:HD22	1:B:63:ILE:CD1	2.50	0.41
1:C:105:ILE:O	1:C:105:ILE:HG23	2.18	0.41
1:C:132:ASP:C	1:C:136:LEU:HG	2.45	0.41
1:D:64:VAL:HG21	1:D:152:HIS:HE1	1.84	0.41
1:A:54:VAL:HG13	1:A:55:SER:N	2.35	0.41
1:B:54:VAL:HG13	1:B:55:SER:N	2.35	0.41
1:C:36:SER:O	1:C:40:GLN:HB2	2.20	0.41
1:C:107:VAL:HG13	1:C:111:CYS:HG	1.85	0.41
1:C:129:GLN:O	1:C:133:LEU:HB2	2.20	0.41
1:C:154:HIS:CE1	1:C:178:ALA:HB3	2.56	0.41
1:C:177:MET:HB3	1:C:200:CYS:CB	2.50	0.41
1:D:11:ARG:HG3	1:D:11:ARG:NH1	2.35	0.41
1:D:77:ARG:HD3	1:D:78:PHE:CE2	2.54	0.41
1:D:179:THR:O	1:D:179:THR:HG22	2.18	0.41
1:D:192:THR:C	1:D:196:VAL:HG23	2.45	0.41
1:A:127:LEU:HA	1:A:130:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASP:OD2	1:A:151:ASP:N	2.53	0.41
1:A:182:LEU:HD13	1:A:182:LEU:HA	1.84	0.41
1:C:65:TYR:CB	1:C:87:ALA:HB1	2.50	0.41
1:C:177:MET:HE2	1:C:203:LEU:CD1	2.50	0.41
1:A:54:VAL:HG12	1:A:59:ILE:HD12	2.02	0.41
1:A:131:GLN:O	1:A:134:VAL:N	2.50	0.41
1:A:159:LYS:HB2	1:A:163:LEU:HD11	2.03	0.41
1:B:34:GLU:HA	1:B:37:TYR:HD2	1.85	0.41
1:B:142:GLN:O	1:B:145:GLY:N	2.49	0.41
1:C:18:GLN:HA	1:C:21:ASN:CB	2.51	0.41
1:D:10:LYS:O	1:D:11:ARG:HG2	2.20	0.41
1:A:21:ASN:ND2	1:B:228:THR:HG22	2.35	0.41
1:A:31:PRO:O	1:A:35:LEU:HB3	2.19	0.41
1:B:46:GLN:HE21	1:B:183:HIS:CE1	2.39	0.41
1:B:137:GLU:O	1:B:137:GLU:HG3	2.20	0.41
1:C:65:TYR:HB3	1:C:87:ALA:HB1	2.02	0.41
1:C:101:LEU:CD2	1:C:134:VAL:HG23	2.50	0.41
1:C:226:ASP:HB2	1:C:229:VAL:HG23	2.02	0.41
1:C:231:LEU:HD23	1:C:232:GLU:N	2.36	0.41
1:C:233:LEU:HD22	1:D:20:GLU:HG2	2.03	0.41
1:D:251:ARG:NH1	1:D:254:ARG:NE	2.68	0.41
1:A:10:LYS:HE3	1:A:10:LYS:HB2	1.21	0.41
1:C:244:ILE:HG22	1:C:248:THR:CG2	2.51	0.41
1:D:124:GLU:OE1	1:D:127:LEU:HD12	2.21	0.41
1:A:10:LYS:O	1:A:11:ARG:HB2	2.21	0.41
1:A:77:ARG:HD3	1:A:78:PHE:CE2	2.55	0.41
1:A:190:GLN:HB3	1:A:191:TYR:CD2	2.56	0.41
1:A:206:LYS:O	1:A:209:ASN:N	2.50	0.41
1:B:203:LEU:CD1	1:B:241:PHE:HB3	2.51	0.41
1:C:170:LEU:CD1	1:C:210:TRP:HB3	2.49	0.41
1:C:192:THR:CG2	1:C:195:VAL:HG23	2.51	0.41
1:C:194:PRO:CA	1:C:225:VAL:HG12	2.51	0.41
1:D:151:ASP:OD2	1:D:151:ASP:N	2.54	0.41
1:D:236:GLU:OE1	1:D:237:LEU:HD21	2.20	0.41
1:A:90:LEU:CD2	1:A:140:ILE:HG23	2.50	0.41
1:C:56:GLN:HE22	1:C:59:ILE:HG22	1.84	0.41
1:C:255:ILE:H	1:C:255:ILE:HG13	1.56	0.41
1:A:32:ASP:O	1:A:35:LEU:HD23	2.20	0.41
1:A:33:LYS:HD2	1:A:33:LYS:HA	1.49	0.41
1:A:99:LYS:HD3	1:A:99:LYS:HA	1.91	0.41
1:A:138:SER:HB2	1:D:134:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:TRP:CH2	1:A:231:LEU:HD13	2.56	0.41
1:A:252:LEU:HD11	1:A:256:TRP:HE1	1.84	0.41
1:B:192:THR:C	1:B:196:VAL:HG23	2.45	0.41
1:C:73:GLN:OE1	1:C:73:GLN:HA	2.17	0.41
1:C:127:LEU:HA	1:C:127:LEU:HD23	1.82	0.41
1:C:153:PRO:HB3	1:C:193:PRO:CA	2.48	0.41
1:C:177:MET:HB3	1:C:200:CYS:HB3	2.02	0.41
1:C:239:HIS:O	1:C:242:LEU:N	2.50	0.41
1:D:42:ALA:HA	1:D:45:LEU:CD1	2.51	0.41
1:D:259:ARG:HA	1:D:262:GLU:CB	2.51	0.41
1:A:74:SER:HB3	1:A:77:ARG:CG	2.41	0.41
1:A:89:PHE:CD1	1:A:104:VAL:HG21	2.56	0.41
1:B:18:GLN:CB	1:B:20:GLU:HG3	2.51	0.41
1:B:19:LEU:HD21	1:B:71:MET:CE	2.51	0.41
1:B:233:LEU:HD21	1:B:237:LEU:HD11	2.03	0.41
1:C:135:ILE:CG2	1:C:136:LEU:HD23	2.51	0.41
1:D:14:PHE:HD1	1:D:18:GLN:NE2	2.19	0.41
1:C:16:ARG:HA	1:C:19:LEU:CD1	2.50	0.40
1:D:26:ARG:CG	1:D:26:ARG:HH11	2.34	0.40
1:D:219:LYS:HB3	1:D:219:LYS:HE2	1.40	0.40
1:A:202:HIS:NE2	1:A:231:LEU:HD11	2.36	0.40
1:B:69:PHE:CE1	1:B:139:ILE:HG22	2.54	0.40
1:A:20:GLU:C	1:A:25:ARG:HE	2.30	0.40
1:A:30:ASP:HB3	1:A:33:LYS:H	1.86	0.40
1:B:19:LEU:HD12	1:B:34:GLU:OE2	2.21	0.40
1:B:251:ARG:HD3	1:B:251:ARG:HA	1.82	0.40
1:C:45:LEU:HG	1:C:88:LEU:HD11	2.04	0.40
1:C:57:LEU:HD13	1:C:57:LEU:HA	1.81	0.40
1:C:161:THR:HG22	1:C:162:GLN:N	2.36	0.40
1:A:219:LYS:CE	1:A:223:GLU:HB3	2.52	0.40
1:B:29:VAL:HG12	1:B:33:LYS:HB3	2.02	0.40
1:C:56:GLN:HE21	1:C:60:ASN:ND2	2.19	0.40
1:C:84:ALA:HB1	1:C:88:LEU:HD13	2.03	0.40
1:C:206:LYS:NZ	2:C:361:HOH:O	2.53	0.40
1:D:51:ARG:HB3	1:D:107:VAL:HG13	2.04	0.40
1:D:54:VAL:HG13	1:D:55:SER:N	2.35	0.40
1:D:135:ILE:HG22	1:D:136:LEU:N	2.35	0.40
1:A:93:LYS:H	1:A:93:LYS:HG3	1.71	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	254/358 (71%)	223 (88%)	26 (10%)	5 (2%)	6	14
1	B	254/358 (71%)	219 (86%)	30 (12%)	5 (2%)	6	14
1	C	254/358 (71%)	186 (73%)	63 (25%)	5 (2%)	6	14
1	D	254/358 (71%)	222 (87%)	26 (10%)	6 (2%)	4	10
All	All	1016/1432 (71%)	850 (84%)	145 (14%)	21 (2%)	5	13

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	THR
1	C	214	VAL
1	D	10	LYS
1	D	215	SER
1	A	38	ARG
1	B	38	ARG
1	C	211	GLU
1	D	28	GLY
1	D	38	ARG
1	B	28	GLY
1	A	28	GLY
1	C	123	SER
1	A	92	ALA
1	A	158	VAL
1	C	161	THR
1	D	158	VAL
1	B	158	VAL
1	C	153	PRO
1	A	72	ILE
1	B	72	ILE
1	D	72	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	227/307 (74%)	138 (61%)	89 (39%)	0	0
1	B	228/307 (74%)	139 (61%)	89 (39%)	0	0
1	C	229/307 (75%)	134 (58%)	95 (42%)	0	0
1	D	228/307 (74%)	136 (60%)	92 (40%)	0	0
All	All	912/1228 (74%)	547 (60%)	365 (40%)	0	0

All (365) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	12	TRP
1	A	15	THR
1	A	16	ARG
1	A	19	LEU
1	A	26	ARG
1	A	30	ASP
1	A	33	LYS
1	A	34	GLU
1	A	35	LEU
1	A	36	SER
1	A	40	GLN
1	A	53	ASN
1	A	54	VAL
1	A	57	LEU
1	A	59	ILE
1	A	63	ILE
1	A	67	HIS
1	A	71	MET
1	A	73	GLN
1	A	76	THR
1	A	77	ARG
1	A	78	PHE
1	A	88	LEU

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Mol	Chain	Res	Type
1	A	93	LYS
1	A	97	GLN
1	A	100	LYS
1	A	101	LEU
1	A	104	VAL
1	A	105	ILE
1	A	106	LYS
1	A	110	THR
1	A	111	CYS
1	A	117	SER
1	A	118	LEU
1	A	121	THR
1	A	122	ARG
1	A	124	GLU
1	A	127	LEU
1	A	129	GLN
1	A	130	VAL
1	A	132	ASP
1	A	133	LEU
1	A	134	VAL
1	A	135	ILE
1	A	137	GLU
1	A	139	ILE
1	A	140	ILE
1	A	141	LEU
1	A	142	GLN
1	A	144	LEU
1	A	147	GLU
1	A	149	THR
1	A	150	ILE
1	A	152	HIS
1	A	155	THR
1	A	157	VAL
1	A	158	VAL
1	A	159	LYS
1	A	161	THR
1	A	168	LYS
1	A	172	GLN
1	A	173	THR
1	A	174	SER
1	A	177	MET
1	A	181	SER

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Mol	Chain	Res	Type
1	A	182	LEU
1	A	184	LEU
1	A	185	THR
1	A	186	THR
1	A	189	LEU
1	A	190	GLN
1	A	203	LEU
1	A	205	CYS
1	A	212	ILE
1	A	214	VAL
1	A	215	SER
1	A	216	THR
1	A	219	LYS
1	A	225	VAL
1	A	228	THR
1	A	230	THR
1	A	233	LEU
1	A	234	LEU
1	A	238	THR
1	A	243	GLN
1	A	251	ARG
1	A	261	CYS
1	A	262	GLU
1	B	10	LYS
1	B	14	PHE
1	B	16	ARG
1	B	18	GLN
1	B	19	LEU
1	B	25	ARG
1	B	26	ARG
1	B	30	ASP
1	B	33	LYS
1	B	35	LEU
1	B	36	SER
1	B	40	GLN
1	B	53	ASN
1	B	54	VAL
1	B	57	LEU
1	B	59	ILE
1	B	63	ILE
1	B	67	HIS
1	B	71	MET

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Mol	Chain	Res	Type
1	B	73	GLN
1	B	76	THR
1	B	78	PHE
1	B	88	LEU
1	B	93	LYS
1	B	96	GLU
1	B	97	GLN
1	B	100	LYS
1	B	101	LEU
1	B	104	VAL
1	B	106	LYS
1	B	110	THR
1	B	111	CYS
1	B	117	SER
1	B	118	LEU
1	B	121	THR
1	B	122	ARG
1	B	124	GLU
1	B	130	VAL
1	B	131	GLN
1	B	132	ASP
1	B	133	LEU
1	B	134	VAL
1	B	135	ILE
1	B	137	GLU
1	B	139	ILE
1	B	141	LEU
1	B	142	GLN
1	B	144	LEU
1	B	146	PHE
1	B	147	GLU
1	B	149	THR
1	B	150	ILE
1	B	152	HIS
1	B	155	THR
1	B	157	VAL
1	B	158	VAL
1	B	159	LYS
1	B	161	THR
1	B	168	LYS
1	B	172	GLN
1	B	173	THR

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Mol	Chain	Res	Type
1	B	174	SER
1	B	177	MET
1	B	181	SER
1	B	182	LEU
1	B	184	LEU
1	B	185	THR
1	B	186	THR
1	B	189	LEU
1	B	190	GLN
1	B	203	LEU
1	B	205	CYS
1	B	212	ILE
1	B	214	VAL
1	B	215	SER
1	B	216	THR
1	B	219	LYS
1	B	225	VAL
1	B	228	THR
1	B	230	THR
1	B	233	LEU
1	B	234	LEU
1	B	238	THR
1	B	243	GLN
1	B	245	LEU
1	B	246	GLU
1	B	247	LYS
1	B	251	ARG
1	B	262	GLU
1	C	10	LYS
1	C	14	PHE
1	C	16	ARG
1	C	18	GLN
1	C	21	ASN
1	C	25	ARG
1	C	26	ARG
1	C	29	VAL
1	C	35	LEU
1	C	36	SER
1	C	44	LEU
1	C	45	LEU
1	C	48	MET
1	C	52	LEU

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Mol	Chain	Res	Type
1	C	54	VAL
1	C	57	LEU
1	C	59	ILE
1	C	61	THR
1	C	64	VAL
1	C	68	ARG
1	C	72	ILE
1	C	73	GLN
1	C	76	THR
1	C	78	PHE
1	C	82	SER
1	C	83	VAL
1	C	88	LEU
1	C	89	PHE
1	C	90	LEU
1	C	94	VAL
1	C	96	GLU
1	C	97	GLN
1	C	99	LYS
1	C	102	GLU
1	C	103	HIS
1	C	104	VAL
1	C	105	ILE
1	C	106	LYS
1	C	107	VAL
1	C	110	THR
1	C	112	LEU
1	C	116	GLU
1	C	118	LEU
1	C	121	THR
1	C	127	LEU
1	C	131	GLN
1	C	132	ASP
1	C	134	VAL
1	C	135	ILE
1	C	136	LEU
1	C	138	SER
1	C	139	ILE
1	C	140	ILE
1	C	141	LEU
1	C	143	THR
1	C	144	LEU

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Mol	Chain	Res	Type
1	C	146	PHE
1	C	147	GLU
1	C	150	ILE
1	C	151	ASP
1	C	154	HIS
1	C	156	HIS
1	C	165	ARG
1	C	168	LYS
1	C	177	MET
1	C	180	ASN
1	C	181	SER
1	C	182	LEU
1	C	185	THR
1	C	186	THR
1	C	199	VAL
1	C	201	ILE
1	C	203	LEU
1	C	205	CYS
1	C	206	LYS
1	C	207	TRP
1	C	208	SER
1	C	212	ILE
1	C	216	THR
1	C	219	LYS
1	C	223	GLU
1	C	226	ASP
1	C	228	THR
1	C	232	GLU
1	C	238	THR
1	C	240	GLU
1	C	243	GLN
1	C	244	ILE
1	C	246	GLU
1	C	247	LYS
1	C	254	ARG
1	C	255	ILE
1	C	256	TRP
1	C	259	ARG
1	C	262	GLU
1	D	9	ASN
1	D	10	LYS
1	D	11	ARG

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Mol	Chain	Res	Type
1	D	16	ARG
1	D	18	GLN
1	D	19	LEU
1	D	20	GLU
1	D	25	ARG
1	D	26	ARG
1	D	30	ASP
1	D	33	LYS
1	D	35	LEU
1	D	36	SER
1	D	40	GLN
1	D	45	LEU
1	D	53	ASN
1	D	54	VAL
1	D	57	LEU
1	D	59	ILE
1	D	63	ILE
1	D	67	HIS
1	D	71	MET
1	D	73	GLN
1	D	76	THR
1	D	77	ARG
1	D	78	PHE
1	D	88	LEU
1	D	93	LYS
1	D	97	GLN
1	D	100	LYS
1	D	101	LEU
1	D	104	VAL
1	D	106	LYS
1	D	110	THR
1	D	111	CYS
1	D	117	SER
1	D	118	LEU
1	D	121	THR
1	D	122	ARG
1	D	124	GLU
1	D	129	GLN
1	D	130	VAL
1	D	131	GLN
1	D	132	ASP
1	D	133	LEU

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Mol	Chain	Res	Type
1	D	134	VAL
1	D	135	ILE
1	D	137	GLU
1	D	139	ILE
1	D	141	LEU
1	D	144	LEU
1	D	146	PHE
1	D	147	GLU
1	D	149	THR
1	D	150	ILE
1	D	152	HIS
1	D	155	THR
1	D	157	VAL
1	D	158	VAL
1	D	159	LYS
1	D	161	THR
1	D	168	LYS
1	D	172	GLN
1	D	173	THR
1	D	174	SER
1	D	177	MET
1	D	181	SER
1	D	182	LEU
1	D	184	LEU
1	D	185	THR
1	D	186	THR
1	D	189	LEU
1	D	203	LEU
1	D	205	CYS
1	D	211	GLU
1	D	212	ILE
1	D	214	VAL
1	D	215	SER
1	D	216	THR
1	D	219	LYS
1	D	225	VAL
1	D	228	THR
1	D	230	THR
1	D	233	LEU
1	D	234	LEU
1	D	238	THR
1	D	243	GLN

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Mol	Chain	Res	Type
1	D	251	ARG
1	D	254	ARG
1	D	259	ARG
1	D	261	CYS
1	D	262	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	21	ASN
1	A	46	GLN
1	A	53	ASN
1	A	56	GLN
1	A	113	HIS
1	A	152	HIS
1	A	156	HIS
1	A	183	HIS
1	A	220	HIS
1	A	250	ASN
1	A	257	ASN
1	B	9	ASN
1	B	21	ASN
1	B	39	GLN
1	B	46	GLN
1	B	50	GLN
1	B	53	ASN
1	B	56	GLN
1	B	97	GLN
1	B	113	HIS
1	B	172	GLN
1	B	180	ASN
1	B	183	HIS
1	B	190	GLN
1	B	202	HIS
1	C	39	GLN
1	C	43	ASN
1	C	56	GLN
1	C	60	ASN
1	C	113	HIS
1	C	129	GLN
1	C	183	HIS

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Mol	Chain	Res	Type
1	C	190	GLN
1	C	257	ASN
1	D	8	ASN
1	D	18	GLN
1	D	40	GLN
1	D	46	GLN
1	D	50	GLN
1	D	53	ASN
1	D	56	GLN
1	D	60	ASN
1	D	97	GLN
1	D	103	HIS
1	D	129	GLN
1	D	142	GLN
1	D	156	HIS
1	D	172	GLN
1	D	190	GLN
1	D	202	HIS
1	D	220	HIS
1	D	239	HIS
1	D	250	ASN
1	D	257	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/358 (71%)	-0.80	0 100 100	23, 60, 69, 76	0
1	B	256/358 (71%)	-0.83	0 100 100	23, 60, 69, 76	0
1	C	256/358 (71%)	-0.82	0 100 100	22, 53, 67, 80	0
1	D	256/358 (71%)	-0.85	0 100 100	24, 61, 69, 76	0
All	All	1024/1432 (71%)	-0.83	0 100 100	22, 59, 69, 80	0

There are no RSRZ outliers to report.

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.