



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:23 AM UTC

PDB ID : 1JQJ / pdb_00001jqj
Title : Mechanism of Processivity Clamp Opening by the Delta Subunit Wrench of the Clamp Loader Complex of E. coli DNA Polymerase III: Structure of the beta-delta complex
Authors : Jeruzalmi, D.; Yurieva, O.; Zhao, Y.; Young, M.; Stewart, J.; Hingorani, M.; O'Donnell, M.; Kuriyan, J.
Deposited on : 2001-08-07
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

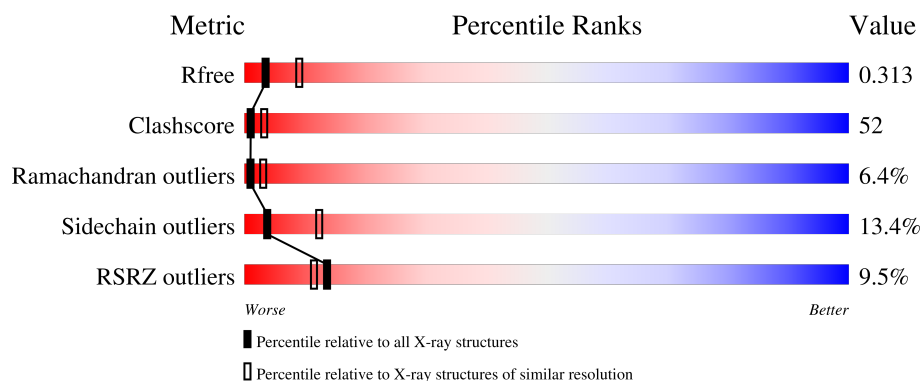
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	366	9% 31% 54% 12% .
1	B	366	13% 33% 53% 13% .
2	C	343	7% 27% 50% 15% .
2	D	343	9% 30% 51% 12% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10860 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 DNA polymerase III, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2837	1780	498	540	19			
1	B	366	Total	C	N	O	S	0	0	0
			2837	1780	498	540	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	ALA	ILE	engineered mutation	UNP P0A988
A	273	ALA	LEU	engineered mutation	UNP P0A988
B	272	ALA	ILE	engineered mutation	UNP P0A988
B	273	ALA	LEU	engineered mutation	UNP P0A988

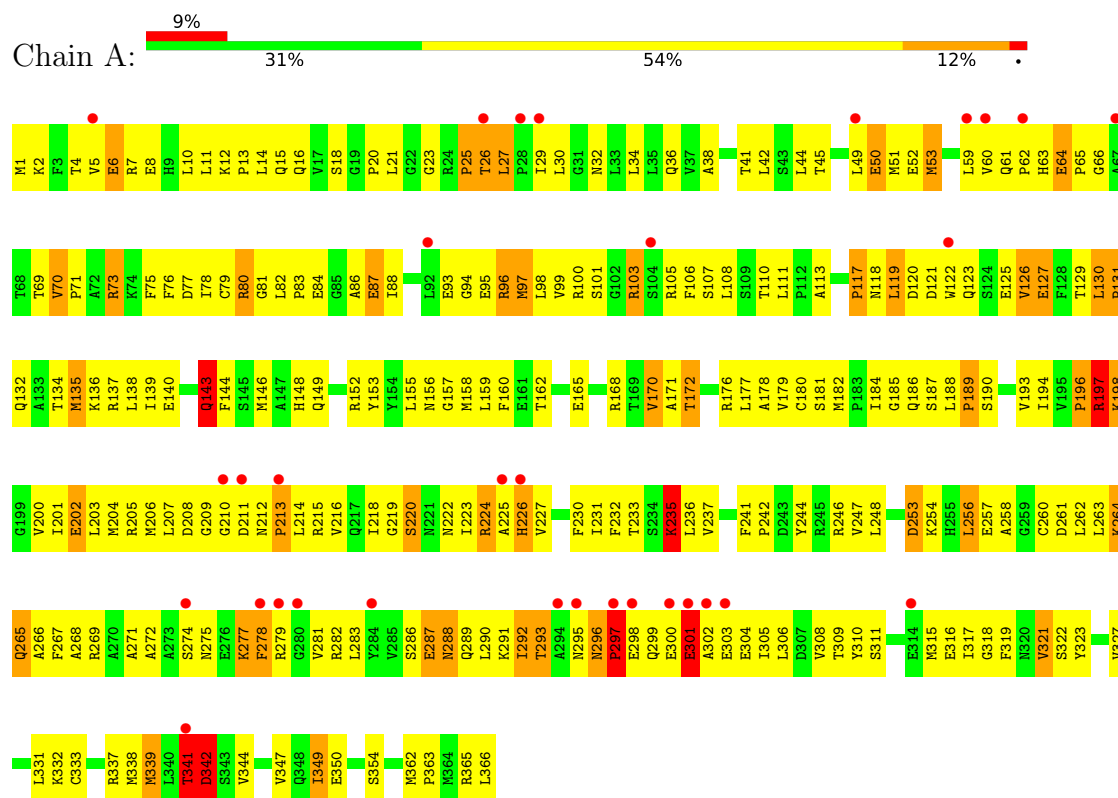
- Molecule 2 is a protein called DNA polymerase III, delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	328	Total	C	N	O	S	0	0	0
			2606	1650	474	472	10			
2	D	325	Total	C	N	O	S	0	0	0
			2580	1632	469	469	10			

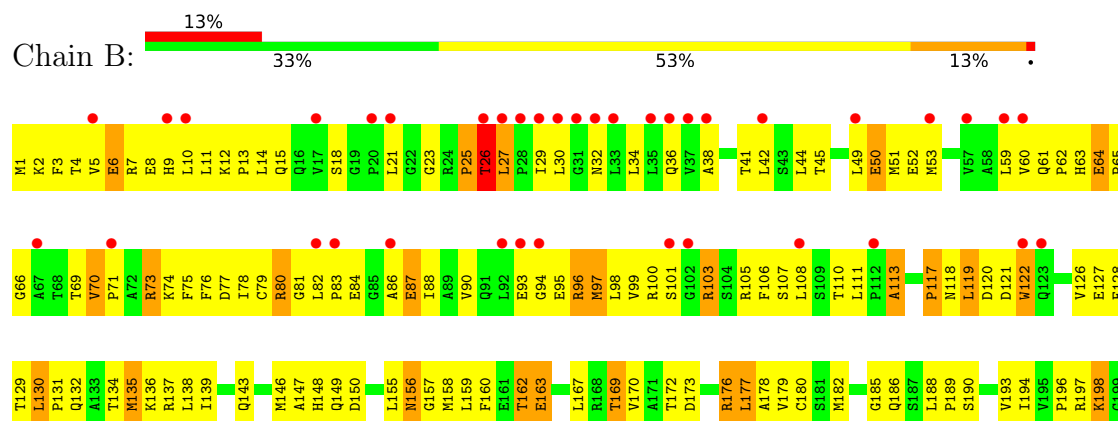
3 Residue-property plots

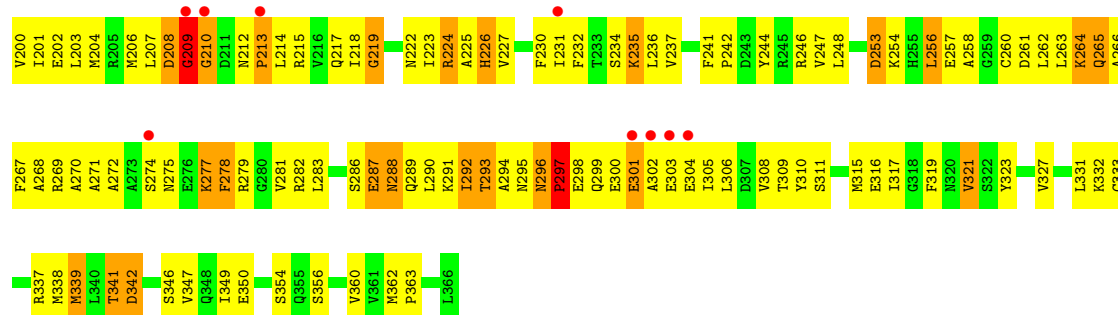
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

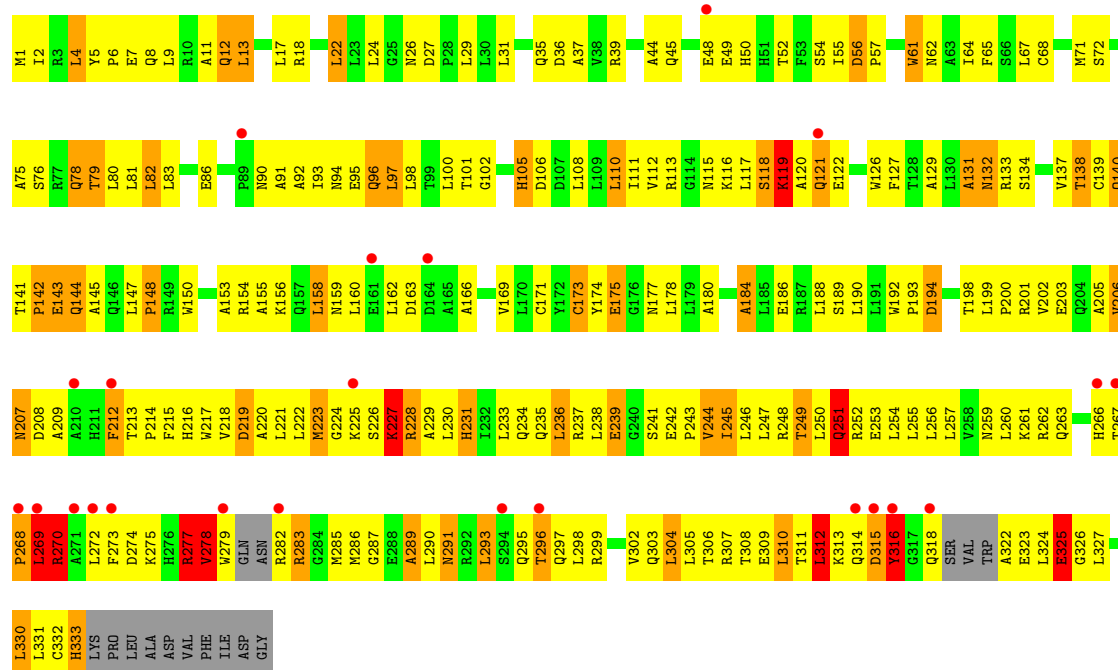


• Molecule 1: DNA polymerase III, beta chain

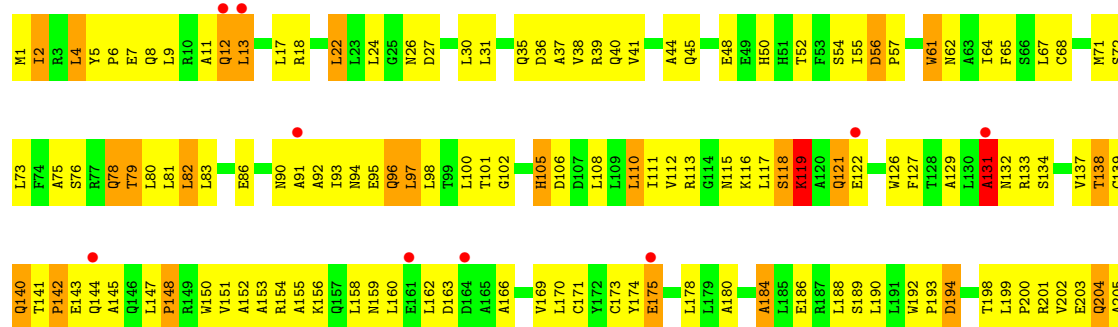


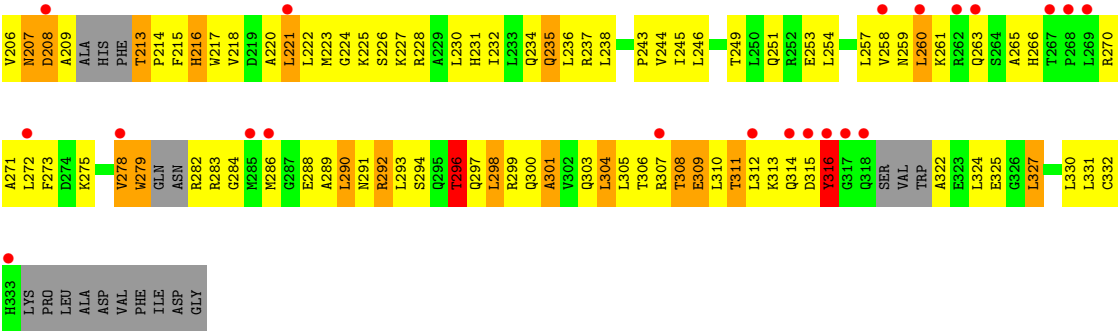


• Molecule 2: DNA polymerase III, delta subunit



• Molecule 2: DNA polymerase III, delta subunit





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.84Å 99.29Å 113.02Å 90.00° 119.17° 90.00°	Depositor
Resolution (Å)	500.00 – 2.90 98.69 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-2.90) 96.5 (98.69-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.88Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.266 , 0.308 0.276 , 0.313	Depositor DCC
R_{free} test set	2188 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10860	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	0.59	1/2886 (0.0%)	1.07	17/3907 (0.4%)
1	B	0.54	1/2886 (0.0%)	1.05	15/3907 (0.4%)
2	C	0.90	3/2649 (0.1%)	1.41	28/3594 (0.8%)
2	D	0.45	0/2620	1.06	17/3553 (0.5%)
All	All	0.64	5/11041 (0.0%)	1.15	77/14961 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	C	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	269	LEU	C-N	-28.53	0.93	1.33
2	C	278	VAL	N-CA	22.34	1.74	1.46
2	C	270	ARG	CB-CG	-9.06	1.25	1.52
1	A	125	GLU	C-N	-6.31	1.30	1.33
1	B	209	GLY	CA-C	-5.51	1.44	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	269	LEU	O-C-N	-27.04	89.37	122.89
2	C	269	LEU	CA-C-N	26.77	172.67	121.54
2	C	269	LEU	C-N-CA	26.77	172.67	121.54
2	C	278	VAL	N-CA-C	18.21	147.22	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	THR	CA-C-N	14.95	146.06	122.59
1	B	341	THR	C-N-CA	14.95	146.06	122.59
1	A	341	THR	CA-C-N	12.20	143.44	121.85
1	A	341	THR	C-N-CA	12.20	143.44	121.85
2	D	314	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	123	GLN	N-CA-C	9.44	123.61	108.41
2	C	325	GLU	N-CA-C	-8.62	102.20	112.89
2	C	238	LEU	N-CA-C	-8.04	102.78	112.59
2	C	278	VAL	N-CA-CB	-7.89	98.22	111.23
1	A	301	GLU	N-CA-C	7.81	116.24	108.75
1	B	209	GLY	O-C-N	-7.74	112.64	122.70
1	B	122	TRP	N-CA-C	-7.55	100.79	110.53
2	C	310	LEU	N-CA-C	-7.53	104.59	114.31
2	C	270	ARG	CA-CB-CG	7.43	128.95	114.10
2	C	268	PRO	N-CA-C	7.14	127.18	112.47
2	C	239	GLU	N-CA-C	-7.06	104.15	114.39
2	D	193	PRO	N-CA-C	-6.96	104.80	113.84
2	C	193	PRO	N-CA-C	-6.87	104.91	113.84
1	B	201	ILE	N-CA-C	-6.81	104.02	110.42
2	D	314	GLN	CG-CD-NE2	6.67	126.41	116.40
2	C	119	LYS	CA-C-N	-6.61	112.25	122.49
2	C	119	LYS	C-N-CA	-6.61	112.25	122.49
1	A	342	ASP	N-CA-CB	6.52	123.65	111.52
2	C	277	ARG	CA-C-N	-6.51	110.24	121.97
2	C	277	ARG	C-N-CA	-6.51	110.24	121.97
1	B	219	GLY	N-CA-C	6.44	119.26	110.69
1	A	143	GLN	N-CA-C	6.23	118.87	111.33
2	D	13	LEU	N-CA-C	-6.16	106.74	114.56
2	C	119	LYS	N-CA-C	6.14	123.88	110.80
1	A	296	ASN	CA-C-N	6.12	127.49	119.84
1	A	296	ASN	C-N-CA	6.12	127.49	119.84
1	A	153	TYR	N-CA-C	6.11	119.57	111.75
2	C	78	GLN	N-CA-C	6.05	118.61	109.23
2	C	296	THR	N-CA-C	-6.05	104.76	111.36
1	A	126	VAL	N-CA-C	-6.04	100.33	107.70
1	B	208	ASP	N-CA-C	-6.04	97.94	110.80
1	B	264	LYS	N-CA-C	-5.83	104.83	111.07
2	D	184	ALA	N-CA-C	-5.83	104.62	110.97
2	C	13	LEU	N-CA-C	-5.76	107.24	114.56
2	C	184	ALA	N-CA-C	-5.76	104.69	110.97
2	D	119	LYS	CA-C-N	-5.76	113.04	122.54
2	D	119	LYS	C-N-CA	-5.76	113.04	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	ASN	CA-C-N	5.72	126.99	119.84
1	B	296	ASN	C-N-CA	5.72	126.99	119.84
2	C	277	ARG	N-CA-C	5.70	122.95	110.80
2	D	301	ALA	N-CA-C	-5.66	105.02	111.07
1	A	196	PRO	N-CA-C	5.65	119.50	110.40
1	A	264	LYS	N-CA-C	-5.64	105.03	111.07
2	D	78	GLN	N-CA-C	5.63	117.96	109.23
2	C	267	THR	N-CA-C	-5.62	97.38	109.81
2	D	324	LEU	N-CA-C	-5.54	105.24	111.28
1	A	235	LYS	N-CA-C	-5.53	103.40	110.53
2	D	122	GLU	N-CA-C	-5.52	106.39	113.02
2	C	315	ASP	N-CA-C	-5.52	105.48	113.21
2	D	119	LYS	N-CA-C	5.51	122.55	110.80
2	C	212	PHE	N-CA-C	-5.50	96.89	107.57
1	B	50	GLU	N-CA-C	-5.50	99.08	110.80
2	C	122	GLU	N-CA-C	-5.43	106.50	113.02
1	B	103	ARG	N-CA-C	-5.43	105.68	114.09
2	D	216	HIS	N-CA-C	-5.39	105.40	111.28
2	D	221	LEU	N-CA-C	-5.27	106.88	113.15
2	D	316	TYR	N-CA-C	5.25	121.97	110.80
1	A	64	GLU	CA-C-N	5.23	126.37	119.84
1	A	64	GLU	C-N-CA	5.23	126.37	119.84
1	A	103	ARG	N-CA-C	-5.21	106.01	114.09
1	A	50	GLU	N-CA-C	-5.17	99.78	110.80
1	B	64	GLU	CA-C-N	5.13	126.25	119.84
1	B	64	GLU	C-N-CA	5.13	126.25	119.84
2	C	142	PRO	N-CA-C	-5.10	101.97	112.47
1	B	113	ALA	N-CA-C	-5.08	107.06	113.20
2	D	131	ALA	N-CA-C	5.02	121.49	110.80
2	C	158	LEU	N-CA-C	-5.01	106.10	113.61
2	D	142	PRO	N-CA-C	-5.01	102.16	112.47

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	341	THR	Peptide
1	B	209	GLY	Mainchain
2	C	269	LEU	Peptide
2	C	277	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2837	0	2849	289	1
1	B	2837	0	2849	272	0
2	C	2606	0	2662	283	2
2	D	2580	0	2641	300	1
All	All	10860	0	11001	1126	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (1126) 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)
2:C:278:VAL:N	2:C:278:VAL:CA	1.74	1.51
2:D:304:LEU:HA	2:D:307:ARG:HD2	1.15	1.11
1:B:136:LYS:HG3	1:B:204:MET:HE1	1.39	1.05
2:D:304:LEU:CA	2:D:307:ARG:HD2	1.85	1.04
1:A:1:MET:HB3	1:A:66:GLY:HA3	1.39	1.04
1:B:266:ALA:HB1	1:B:292:ILE:HG21	1.40	1.02
1:A:266:ALA:HB1	1:A:292:ILE:HG21	1.38	1.01
2:D:96:GLN:HA	2:D:96:GLN:HE21	1.25	1.00
2:D:304:LEU:HA	2:D:307:ARG:CD	1.91	1.00
1:B:1:MET:HB3	1:B:66:GLY:HA3	1.40	0.99
2:C:166:ALA:HB1	2:C:202:VAL:HG21	1.44	0.99
2:C:96:GLN:HA	2:C:96:GLN:HE21	1.27	0.96
1:B:246:ARG:NH1	1:B:246:ARG:HB3	1.83	0.94
2:C:90:ASN:ND2	2:C:91:ALA:H	1.65	0.94
1:A:126:VAL:CG1	1:A:218:ILE:HB	1.96	0.94
1:A:246:ARG:HB3	1:A:246:ARG:NH1	1.83	0.93
1:B:283:LEU:HD22	1:B:290:LEU:HD11	1.50	0.93
2:D:90:ASN:ND2	2:D:91:ALA:H	1.67	0.93
1:B:51:MET:HE1	1:B:198:LYS:HB3	1.49	0.92
2:D:300:GLN:HE21	2:D:307:ARG:HH22	1.13	0.92
2:D:292:ARG:HB2	2:D:292:ARG:NH1	1.84	0.92
2:C:86:GLU:CD	2:C:86:GLU:H	1.78	0.92
1:A:165:GLU:HG2	1:A:187:SER:HA	1.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:GLU:H	2:D:86:GLU:CD	1.77	0.91
2:D:90:ASN:HB3	2:D:93:ILE:HG12	1.50	0.91
2:D:304:LEU:HD11	2:D:327:LEU:HD22	1.51	0.91
1:B:208:ASP:O	1:B:210:GLY:N	2.03	0.90
1:A:246:ARG:HB3	1:A:246:ARG:HH11	1.36	0.90
2:C:140:GLN:HE21	2:C:140:GLN:HA	1.37	0.90
1:A:362:MET:HE3	2:C:71:MET:HB3	1.52	0.89
1:B:246:ARG:HB3	1:B:246:ARG:HH11	1.36	0.89
2:D:311:THR:HG22	2:D:315:ASP:HB2	1.52	0.88
1:A:283:LEU:HD22	1:A:290:LEU:HD11	1.52	0.88
2:D:223:MET:HE2	2:D:289:ALA:HA	1.55	0.88
2:D:227:LYS:H	2:D:227:LYS:HD2	1.38	0.88
2:C:311:THR:HA	2:C:315:ASP:OD2	1.74	0.88
1:A:136:LYS:HG3	1:A:204:MET:HE1	1.53	0.88
2:C:90:ASN:HB3	2:C:93:ILE:HG12	1.54	0.88
2:D:1:MET:HB2	2:D:131:ALA:O	1.74	0.88
2:C:225:LYS:O	2:C:229:ALA:HB2	1.74	0.87
1:B:122:TRP:CD1	1:B:122:TRP:H	1.85	0.87
2:C:1:MET:HB2	2:C:131:ALA:O	1.75	0.87
1:B:197:ARG:HG2	1:B:198:LYS:HE2	1.56	0.87
2:C:163:ASP:OD1	2:C:198:THR:HA	1.75	0.87
2:D:163:ASP:OD1	2:D:198:THR:HA	1.74	0.87
1:A:226:HIS:CD2	1:A:226:HIS:H	1.91	0.87
2:D:39:ARG:HE	2:D:79:THR:HG21	1.39	0.87
1:B:170:VAL:HG12	1:B:179:VAL:HG13	1.54	0.86
2:C:39:ARG:HE	2:C:79:THR:HG21	1.41	0.85
2:D:253:GLU:HB3	2:D:286:MET:HE1	1.55	0.85
2:C:225:LYS:HE2	2:C:228:ARG:HB2	1.58	0.84
1:A:177:LEU:HD21	1:A:179:VAL:HG23	1.59	0.84
2:D:118:SER:HB2	2:D:121:GLN:HE21	1.43	0.83
1:A:226:HIS:H	1:A:226:HIS:HD2	1.26	0.83
2:C:118:SER:HB2	2:C:121:GLN:HE21	1.42	0.83
2:D:225:LYS:HB3	2:D:227:LYS:HD3	1.61	0.83
2:D:292:ARG:HB2	2:D:292:ARG:HH11	1.41	0.83
2:C:270:ARG:O	2:C:274:ASP:OD2	1.97	0.83
1:A:126:VAL:HG12	1:A:218:ILE:HB	1.62	0.82
2:C:140:GLN:HA	2:C:140:GLN:NE2	1.93	0.82
2:C:50:HIS:ND1	2:C:79:THR:HB	1.95	0.82
2:D:225:LYS:HB2	2:D:228:ARG:HE	1.45	0.82
2:C:306:THR:O	2:C:310:LEU:HG	1.80	0.81
2:C:1:MET:HE3	2:C:131:ALA:HA	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:277:ARG:C	2:C:278:VAL:CA	2.53	0.81
2:C:307:ARG:HA	2:C:310:LEU:HD12	1.63	0.81
2:C:22:LEU:HD12	2:C:112:VAL:HB	1.62	0.81
1:B:2:LYS:HG2	1:B:64:GLU:HB2	1.63	0.81
2:C:141:THR:HG22	2:C:142:PRO:O	1.81	0.81
1:A:51:MET:HE1	1:A:198:LYS:HB3	1.63	0.80
2:D:39:ARG:HH21	2:D:79:THR:HG22	1.45	0.80
2:D:50:HIS:ND1	2:D:79:THR:HB	1.97	0.80
2:D:221:LEU:C	2:D:223:MET:H	1.90	0.80
2:D:308:THR:HA	2:D:311:THR:OG1	1.82	0.80
1:A:222:ASN:HD21	1:A:235:LYS:NZ	1.79	0.79
2:D:1:MET:HE3	2:D:131:ALA:HA	1.63	0.79
2:D:223:MET:CE	2:D:289:ALA:HA	2.12	0.79
2:D:56:ASP:HB2	2:D:57:PRO:HD2	1.64	0.79
1:A:2:LYS:HG2	1:A:64:GLU:HB2	1.63	0.79
2:C:39:ARG:HH21	2:C:79:THR:HG22	1.47	0.78
1:A:130:LEU:HD21	1:A:135:MET:HB2	1.65	0.78
1:A:122:TRP:HZ3	1:A:219:GLY:HA3	1.46	0.78
2:C:296:THR:HG23	2:C:299:ARG:HH12	1.47	0.78
2:D:141:THR:HG22	2:D:142:PRO:O	1.82	0.78
1:A:100:ARG:HG2	1:A:105:ARG:HB3	1.66	0.78
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.64	0.78
1:A:256:LEU:HD13	1:A:308:VAL:HG21	1.65	0.78
1:A:165:GLU:OE2	1:B:60:VAL:HB	1.84	0.78
2:C:282:ARG:O	2:C:285:MET:N	2.15	0.77
1:A:262:LEU:HG	1:A:306:LEU:HD21	1.66	0.77
1:B:218:ILE:HG22	1:B:219:GLY:H	1.49	0.77
2:C:56:ASP:HB2	2:C:57:PRO:HD2	1.66	0.77
1:A:156:ASN:O	1:A:197:ARG:HG2	1.85	0.77
1:A:224:ARG:HD2	1:A:226:HIS:NE2	2.00	0.77
2:C:202:VAL:O	2:C:206:VAL:HG23	1.85	0.77
1:B:100:ARG:HG2	1:B:105:ARG:HB3	1.65	0.77
1:B:214:LEU:CD1	1:B:225:ALA:HB1	2.15	0.77
2:D:22:LEU:HD12	2:D:112:VAL:HB	1.67	0.77
2:C:278:VAL:H	2:C:278:VAL:HG13	1.50	0.76
1:A:222:ASN:HD21	1:A:235:LYS:HZ1	1.30	0.76
2:D:199:LEU:HB3	2:D:200:PRO:HD3	1.68	0.76
1:A:152:ARG:HD3	2:C:48:GLU:HG3	1.69	0.75
2:C:199:LEU:HB3	2:C:200:PRO:HD3	1.68	0.75
1:A:122:TRP:CZ3	1:A:219:GLY:HA3	2.21	0.75
2:C:242:GLU:O	2:C:245:ILE:HG22	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:LEU:HD23	2:D:294:SER:N	2.02	0.75
1:B:279:ARG:HD2	1:B:297:PRO:HG2	1.69	0.74
1:A:118:ASN:O	1:A:120:ASP:N	2.20	0.74
1:A:23:GLY:C	1:A:25:PRO:HD3	2.12	0.74
1:B:308:VAL:HG22	1:B:309:THR:N	2.03	0.74
2:D:140:GLN:HE21	2:D:140:GLN:HA	1.53	0.74
2:D:249:THR:O	2:D:253:GLU:HG2	1.87	0.74
2:C:287:GLY:O	2:C:291:ASN:HB2	1.88	0.74
1:A:129:THR:H	1:A:186:GLN:HE22	1.34	0.74
1:B:256:LEU:HD13	1:B:308:VAL:HG21	1.68	0.74
2:D:199:LEU:O	2:D:203:GLU:HG2	1.87	0.74
2:D:254:LEU:HD21	2:D:301:ALA:HB3	1.69	0.74
1:A:69:THR:HB	1:A:111:LEU:O	1.88	0.73
2:D:225:LYS:HD3	2:D:228:ARG:HH21	1.53	0.73
2:D:300:GLN:NE2	2:D:307:ARG:HH22	1.85	0.73
1:B:23:GLY:C	1:B:25:PRO:HD3	2.12	0.73
2:C:173:CYS:HB3	2:C:212:PHE:HE1	1.53	0.73
1:B:176:ARG:HH11	1:B:176:ARG:HG2	1.53	0.73
1:B:289:GLN:OE1	1:B:291:LYS:HE3	1.88	0.73
2:C:278:VAL:N	2:C:278:VAL:CB	2.50	0.73
1:A:53:MET:HE1	1:A:230:PHE:HB3	1.69	0.73
1:B:281:VAL:HG23	1:B:321:VAL:HG22	1.71	0.73
1:B:282:ARG:HB2	1:B:295:ASN:HB2	1.71	0.73
2:D:140:GLN:HA	2:D:140:GLN:NE2	2.02	0.73
1:A:308:VAL:HG22	1:A:309:THR:N	2.04	0.73
1:B:262:LEU:HG	1:B:306:LEU:HD21	1.71	0.73
2:C:118:SER:HB2	2:C:121:GLN:NE2	2.03	0.73
1:A:177:LEU:HD13	1:A:247:VAL:HG21	1.71	0.73
1:A:281:VAL:HG23	1:A:321:VAL:HG22	1.69	0.73
2:D:118:SER:OG	2:D:121:GLN:HG2	1.89	0.73
2:D:221:LEU:HD23	2:D:221:LEU:O	1.89	0.73
1:A:363:PRO:HG2	2:C:71:MET:HE3	1.70	0.72
1:B:218:ILE:HG22	1:B:219:GLY:N	2.04	0.72
2:D:118:SER:HB2	2:D:121:GLN:NE2	2.03	0.72
2:C:118:SER:OG	2:C:121:GLN:HG2	1.89	0.72
2:C:81:LEU:HD12	2:C:111:ILE:HB	1.69	0.72
1:A:289:GLN:OE1	1:A:291:LYS:HE3	1.88	0.72
1:A:282:ARG:HB2	1:A:295:ASN:HB2	1.70	0.72
2:C:80:LEU:HD23	2:C:110:LEU:HD12	1.72	0.72
2:D:299:ARG:NH1	2:D:299:ARG:HB3	2.04	0.72
1:A:230:PHE:C	1:A:231:ILE:HD12	2.15	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:HD2	1:A:297:PRO:HG2	1.71	0.72
2:D:80:LEU:HD23	2:D:110:LEU:HD12	1.70	0.71
1:B:293:THR:HB	1:B:303:GLU:HB3	1.71	0.71
1:A:293:THR:HB	1:A:303:GLU:HB3	1.72	0.71
2:D:260:LEU:HD23	2:D:272:LEU:HD23	1.72	0.71
2:D:303:GLN:O	2:D:307:ARG:HG3	1.91	0.71
1:B:208:ASP:O	1:B:208:ASP:OD1	2.09	0.71
2:C:222:LEU:HD12	2:C:285:MET:HE3	1.72	0.71
1:A:308:VAL:HG22	1:A:309:THR:H	1.56	0.70
1:A:82:LEU:HB3	1:A:83:PRO:HD2	1.74	0.70
1:B:208:ASP:C	1:B:210:GLY:H	2.00	0.70
1:B:308:VAL:HG22	1:B:309:THR:H	1.57	0.70
2:C:26:ASN:H	2:C:140:GLN:HE22	1.37	0.70
2:C:257:LEU:HD23	2:C:260:LEU:HD12	1.73	0.69
2:D:166:ALA:HB1	2:D:202:VAL:HG21	1.74	0.69
1:B:277:LYS:HE3	2:D:62:ASN:HD21	1.56	0.69
2:C:278:VAL:N	2:C:278:VAL:HA	2.01	0.69
2:D:203:GLU:C	2:D:205:ALA:H	2.00	0.69
1:B:69:THR:HB	1:B:111:LEU:O	1.91	0.69
1:A:143:GLN:O	1:A:146:MET:HG2	1.91	0.69
2:C:96:GLN:HE21	2:C:96:GLN:CA	2.03	0.69
2:C:260:LEU:HB3	2:C:290:LEU:HD11	1.73	0.69
1:A:226:HIS:CD2	1:A:226:HIS:N	2.60	0.69
1:B:12:LYS:HB2	1:B:13:PRO:HD3	1.75	0.69
1:B:103:ARG:HH11	1:B:105:ARG:NH1	1.92	0.69
2:C:90:ASN:ND2	2:C:91:ALA:N	2.41	0.68
2:C:251:GLN:HB2	2:C:305:LEU:HD21	1.74	0.68
2:D:97:LEU:O	2:D:101:THR:HG23	1.93	0.68
2:D:253:GLU:HB3	2:D:286:MET:CE	2.22	0.68
1:B:82:LEU:HB3	1:B:83:PRO:HD2	1.75	0.68
1:B:138:LEU:HD21	1:B:182:MET:HG2	1.74	0.68
1:A:103:ARG:HH11	1:A:105:ARG:NH1	1.92	0.68
2:C:225:LYS:HE2	2:C:228:ARG:CB	2.23	0.68
2:D:26:ASN:H	2:D:140:GLN:HE22	1.42	0.68
2:C:140:GLN:HE21	2:C:140:GLN:CA	2.03	0.68
2:C:11:ALA:C	2:C:13:LEU:H	2.01	0.68
1:B:2:LYS:HE2	1:B:64:GLU:HG3	1.76	0.67
2:D:35:GLN:O	2:D:39:ARG:HG3	1.94	0.67
1:A:2:LYS:HE2	1:A:64:GLU:HG3	1.75	0.67
2:D:81:LEU:HD12	2:D:111:ILE:HB	1.75	0.67
2:C:247:LEU:HD11	2:C:308:THR:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:306:THR:O	2:D:310:LEU:HG	1.93	0.67
1:B:196:PRO:O	1:B:200:VAL:HG23	1.94	0.67
2:D:223:MET:SD	2:D:292:ARG:HB3	2.34	0.67
2:D:300:GLN:HE21	2:D:307:ARG:NH2	1.91	0.67
2:C:225:LYS:O	2:C:229:ALA:CB	2.42	0.67
1:A:12:LYS:HB2	1:A:13:PRO:HD3	1.75	0.67
2:D:96:GLN:HE21	2:D:96:GLN:CA	2.01	0.67
1:A:148:HIS:ND1	1:A:149:GLN:HG3	2.10	0.67
1:A:16:GLN:HG2	1:A:230:PHE:CD2	2.29	0.67
1:A:130:LEU:HD22	1:A:131:PRO:O	1.95	0.67
2:D:273:PHE:CZ	2:D:283:ARG:HG3	2.30	0.67
1:A:315:MET:HE2	1:A:317:ILE:HB	1.76	0.66
1:B:317:ILE:HD11	1:B:363:PRO:HB3	1.77	0.66
2:C:133:ARG:O	2:C:133:ARG:HG2	1.95	0.66
1:B:315:MET:HE2	1:B:317:ILE:HB	1.76	0.66
2:D:96:GLN:HA	2:D:96:GLN:NE2	2.07	0.66
1:B:83:PRO:HG2	1:B:86:ALA:HB2	1.78	0.66
2:C:65:PHE:HE2	2:C:100:LEU:HB2	1.59	0.66
2:C:166:ALA:HB1	2:C:202:VAL:CG2	2.22	0.66
1:B:38:ALA:O	1:B:41:THR:HG22	1.96	0.66
1:B:118:ASN:O	1:B:120:ASP:N	2.29	0.66
2:C:278:VAL:N	2:C:278:VAL:CG1	2.58	0.66
2:D:39:ARG:NE	2:D:79:THR:HG21	2.11	0.66
1:A:292:ILE:HD13	1:A:292:ILE:C	2.21	0.66
1:B:292:ILE:C	1:B:292:ILE:HD13	2.20	0.66
1:A:288:ASN:N	1:A:288:ASN:HD22	1.92	0.66
2:C:217:TRP:NE1	2:C:233:LEU:HD13	2.10	0.66
1:A:317:ILE:HD11	1:A:363:PRO:HB3	1.78	0.66
1:B:230:PHE:O	1:B:231:ILE:HD12	1.96	0.66
2:C:186:GLU:O	2:C:189:SER:HB3	1.96	0.65
2:D:186:GLU:O	2:D:189:SER:HB3	1.96	0.65
1:B:176:ARG:HG2	1:B:176:ARG:NH1	2.11	0.65
1:B:230:PHE:C	1:B:231:ILE:HD12	2.21	0.65
2:D:174:TYR:CD2	2:D:180:ALA:HB1	2.32	0.65
1:B:194:ILE:CG2	1:B:237:VAL:HB	2.26	0.65
2:C:231:HIS:C	2:C:231:HIS:CD2	2.75	0.65
2:C:97:LEU:O	2:C:101:THR:HG23	1.95	0.65
2:C:174:TYR:CD2	2:C:180:ALA:HB1	2.32	0.65
2:C:145:ALA:O	2:C:148:PRO:HD2	1.96	0.65
2:C:96:GLN:HA	2:C:96:GLN:NE2	2.08	0.65
2:C:86:GLU:CD	2:C:86:GLU:N	2.52	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:247:LEU:CD1	2:C:309:GLU:HB3	2.27	0.65
2:D:65:PHE:HE2	2:D:100:LEU:HB2	1.60	0.65
2:D:204:GLN:HG2	2:D:204:GLN:O	1.97	0.65
1:A:83:PRO:HG2	1:A:86:ALA:HB2	1.77	0.65
1:A:184:ILE:HG13	1:A:186:GLN:H	1.61	0.65
2:C:26:ASN:H	2:C:140:GLN:NE2	1.94	0.65
1:A:288:ASN:HD22	1:A:288:ASN:H	1.46	0.64
2:D:11:ALA:C	2:D:13:LEU:H	2.04	0.64
2:D:304:LEU:HA	2:D:307:ARG:CG	2.27	0.64
1:A:60:VAL:HG23	1:A:61:GLN:HG3	1.80	0.64
2:D:225:LYS:CB	2:D:227:LYS:HD3	2.27	0.64
1:A:286:SER:O	1:A:287:GLU:C	2.40	0.64
1:B:51:MET:HB2	1:B:232:PHE:HE1	1.62	0.64
1:B:97:MET:HE3	1:B:97:MET:HA	1.78	0.64
2:C:225:LYS:HE2	2:C:228:ARG:HG3	1.80	0.64
1:B:34:LEU:HB3	1:B:45:THR:HB	1.80	0.64
2:D:133:ARG:O	2:D:133:ARG:HG2	1.96	0.64
2:C:173:CYS:HB3	2:C:212:PHE:CE1	2.33	0.64
2:C:214:PRO:HB3	2:C:246:LEU:CD2	2.27	0.64
2:C:260:LEU:CB	2:C:290:LEU:HD11	2.28	0.64
2:D:90:ASN:ND2	2:D:91:ALA:N	2.44	0.64
2:D:234:GLN:O	2:D:238:LEU:HG	1.98	0.64
1:B:137:ARG:HH22	1:B:356:SER:HB2	1.62	0.63
1:A:38:ALA:O	1:A:41:THR:HG22	1.98	0.63
2:D:2:ILE:HD12	2:D:2:ILE:N	2.14	0.63
1:B:103:ARG:NH1	1:B:105:ARG:HH12	1.97	0.63
2:D:26:ASN:H	2:D:140:GLN:NE2	1.97	0.63
1:B:172:THR:HB	1:B:177:LEU:HD12	1.80	0.63
2:C:35:GLN:O	2:C:39:ARG:HG3	1.98	0.63
2:C:278:VAL:N	2:C:278:VAL:HG13	2.13	0.63
1:B:60:VAL:HG23	1:B:61:GLN:HG3	1.79	0.63
1:B:193:VAL:HB	1:B:236:LEU:HD13	1.80	0.63
2:C:2:ILE:N	2:C:2:ILE:HD12	2.13	0.63
2:C:247:LEU:HD12	2:C:309:GLU:HB3	1.80	0.63
2:C:192:TRP:CE2	2:C:201:ARG:HD3	2.33	0.63
1:A:50:GLU:OE1	1:A:51:MET:HE2	1.98	0.62
2:D:306:THR:O	2:D:309:GLU:HG3	1.99	0.62
2:D:227:LYS:H	2:D:227:LYS:CD	2.10	0.62
1:B:132:GLN:NE2	1:B:227:VAL:HG13	2.14	0.62
1:B:288:ASN:N	1:B:288:ASN:HD22	1.96	0.62
2:D:225:LYS:HB2	2:D:228:ARG:NE	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:272:LEU:HA	2:D:275:LYS:HB2	1.82	0.62
1:B:23:GLY:O	1:B:25:PRO:HD3	1.99	0.62
1:B:170:VAL:CG1	1:B:179:VAL:HG13	2.29	0.62
2:C:39:ARG:NE	2:C:79:THR:HG21	2.11	0.62
2:D:278:VAL:HG13	2:D:282:ARG:NH1	2.15	0.62
2:D:207:ASN:HD22	2:D:208:ASP:H	1.47	0.62
2:D:288:GLU:HG2	2:D:292:ARG:NH1	2.15	0.62
2:D:257:LEU:HA	2:D:290:LEU:HD21	1.82	0.62
1:A:103:ARG:NH1	1:A:105:ARG:HH12	1.97	0.62
2:C:177:ASN:HD22	2:C:241:SER:HB2	1.64	0.62
1:A:97:MET:HE3	1:A:97:MET:HA	1.80	0.61
2:D:145:ALA:O	2:D:148:PRO:HD2	1.99	0.61
2:D:304:LEU:C	2:D:304:LEU:HD12	2.25	0.61
1:A:23:GLY:O	1:A:25:PRO:HD3	2.00	0.61
2:C:282:ARG:O	2:C:283:ARG:C	2.42	0.61
2:D:221:LEU:C	2:D:223:MET:N	2.54	0.61
2:D:221:LEU:HD21	2:D:331:LEU:HD12	1.83	0.61
1:B:50:GLU:OE1	1:B:51:MET:HE2	1.99	0.61
2:D:312:LEU:O	2:D:316:TYR:HD2	1.83	0.61
1:B:73:ARG:HE	1:B:73:ARG:HA	1.65	0.61
1:B:82:LEU:HD13	1:B:101:SER:CB	2.31	0.61
2:C:225:LYS:HG3	2:C:228:ARG:HG3	1.81	0.61
2:D:203:GLU:O	2:D:205:ALA:N	2.34	0.61
1:A:7:ARG:HG2	1:A:7:ARG:O	2.01	0.61
2:D:330:LEU:HD13	2:D:330:LEU:O	2.00	0.61
1:B:286:SER:O	1:B:287:GLU:C	2.42	0.61
2:C:150:TRP:CH2	2:C:178:LEU:HD12	2.36	0.61
2:C:273:PHE:HZ	2:C:286:MET:HB2	1.66	0.61
1:A:73:ARG:HE	1:A:73:ARG:HA	1.66	0.61
2:D:313:LYS:HA	2:D:316:TYR:CD2	2.36	0.61
1:A:111:LEU:N	1:A:111:LEU:HD12	2.16	0.61
2:D:101:THR:HG21	2:D:126:TRP:HB2	1.82	0.61
2:D:259:ASN:C	2:D:261:LYS:H	2.09	0.61
1:A:224:ARG:HD2	1:A:226:HIS:CD2	2.36	0.60
1:B:51:MET:CE	1:B:198:LYS:HB3	2.27	0.60
2:C:101:THR:HG21	2:C:126:TRP:HB2	1.82	0.60
1:A:137:ARG:NH1	1:A:180:CYS:SG	2.74	0.60
1:A:215:ARG:NH2	1:A:226:HIS:ND1	2.48	0.60
1:B:362:MET:HE2	2:D:72:SER:O	2.01	0.60
2:D:140:GLN:HE21	2:D:140:GLN:CA	2.13	0.60
2:D:296:THR:HA	2:D:299:ARG:HH12	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLY:O	1:B:210:GLY:O	2.19	0.60
2:C:256:LEU:HA	2:C:259:ASN:ND2	2.16	0.60
1:A:257:GLU:O	1:A:308:VAL:HG23	2.01	0.60
1:B:7:ARG:O	1:B:7:ARG:HG2	2.02	0.60
2:D:169:VAL:HG21	2:D:199:LEU:HD11	1.82	0.60
1:A:1:MET:HB3	1:A:66:GLY:CA	2.25	0.60
1:A:82:LEU:HD13	1:A:101:SER:CB	2.32	0.60
2:D:297:GLN:CD	2:D:297:GLN:H	2.09	0.60
1:A:53:MET:CE	1:A:230:PHE:HB3	2.32	0.60
1:A:60:VAL:HG23	1:A:61:GLN:H	1.66	0.60
2:C:1:MET:CB	2:C:131:ALA:O	2.50	0.60
2:D:86:GLU:CD	2:D:86:GLU:N	2.52	0.60
2:D:150:TRP:CH2	2:D:178:LEU:HD12	2.37	0.60
2:C:169:VAL:HG21	2:C:199:LEU:HD11	1.82	0.60
2:D:309:GLU:OE1	2:D:310:LEU:HD23	2.02	0.60
1:A:203:LEU:HD12	1:A:203:LEU:O	2.01	0.59
2:D:243:PRO:HA	2:D:246:LEU:HD12	1.84	0.59
2:C:255:LEU:HD23	2:C:259:ASN:HD21	1.67	0.59
2:D:223:MET:HE1	2:D:292:ARG:HB2	1.84	0.59
1:A:203:LEU:O	1:A:207:LEU:HG	2.01	0.59
1:A:34:LEU:HB3	1:A:45:THR:HB	1.83	0.59
2:C:217:TRP:CE2	2:C:233:LEU:HD13	2.37	0.59
2:C:226:SER:O	2:C:230:LEU:HD13	2.03	0.59
1:A:349:ILE:HD12	1:A:349:ILE:N	2.17	0.59
1:B:269:ARG:HD2	1:B:304:GLU:OE1	2.03	0.59
1:B:288:ASN:HD22	1:B:288:ASN:H	1.49	0.59
2:C:27:ASP:OD2	2:C:178:LEU:HD23	2.01	0.59
2:D:90:ASN:O	2:D:94:ASN:ND2	2.34	0.59
1:A:14:LEU:HD21	1:A:76:PHE:HA	1.85	0.59
2:C:243:PRO:C	2:C:245:ILE:H	2.09	0.59
1:A:265:GLN:O	1:A:266:ALA:C	2.46	0.59
1:B:185:GLY:O	1:B:186:GLN:HG3	2.03	0.59
2:C:225:LYS:CE	2:C:228:ARG:HB2	2.31	0.59
2:C:306:THR:HG22	2:C:310:LEU:HD11	1.83	0.59
1:A:260:CYS:O	1:A:264:LYS:HG3	2.03	0.59
1:B:60:VAL:HG23	1:B:61:GLN:H	1.67	0.59
1:B:223:ILE:HG22	1:B:236:LEU:HD21	1.85	0.59
1:B:257:GLU:O	1:B:308:VAL:HG23	2.03	0.59
1:A:27:LEU:HG	1:A:30:LEU:HD12	1.85	0.59
1:A:36:GLN:O	1:A:42:LEU:HD12	2.03	0.59
2:D:4:LEU:HD21	2:D:12:GLN:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:ASN:HD22	2:D:208:ASP:N	2.00	0.59
1:A:32:ASN:HB3	1:A:69:THR:HG22	1.84	0.58
1:B:32:ASN:HB3	1:B:69:THR:HG22	1.84	0.58
2:C:311:THR:O	2:C:315:ASP:N	2.36	0.58
2:D:39:ARG:HH21	2:D:79:THR:CG2	2.13	0.58
1:A:168:ARG:HG3	1:A:168:ARG:O	2.03	0.58
1:B:128:PHE:HE2	1:B:218:ILE:HD11	1.67	0.58
1:B:214:LEU:HD11	1:B:225:ALA:CB	2.32	0.58
2:C:118:SER:CB	2:C:121:GLN:HE21	2.15	0.58
2:C:296:THR:CG2	2:C:299:ARG:HH12	2.16	0.58
2:D:327:LEU:O	2:D:331:LEU:HG	2.02	0.58
1:A:165:GLU:HG2	1:A:187:SER:CA	2.31	0.58
2:C:231:HIS:NE2	2:C:235:GLN:CD	2.61	0.58
1:B:14:LEU:HD21	1:B:76:PHE:HA	1.84	0.58
1:A:63:HIS:O	1:A:64:GLU:HG2	2.04	0.58
1:B:103:ARG:HH11	1:B:105:ARG:HH12	1.50	0.58
2:C:255:LEU:HD23	2:C:255:LEU:C	2.29	0.58
1:A:53:MET:HE1	1:A:230:PHE:CB	2.33	0.58
1:A:88:ILE:HD12	1:A:88:ILE:N	2.19	0.58
1:B:135:MET:HE1	1:B:160:PHE:HE2	1.68	0.58
1:B:150:ASP:O	1:B:156:ASN:ND2	2.36	0.58
2:D:293:LEU:HD22	2:D:298:LEU:HD13	1.85	0.58
1:A:171:ALA:C	1:A:172:THR:HG22	2.27	0.58
1:A:196:PRO:O	1:A:200:VAL:HG23	2.04	0.58
1:B:129:THR:H	1:B:186:GLN:HE22	1.52	0.58
2:C:305:LEU:C	2:C:305:LEU:HD23	2.28	0.58
2:D:118:SER:CB	2:D:121:GLN:HE21	2.16	0.58
2:C:90:ASN:O	2:C:94:ASN:ND2	2.37	0.57
2:C:255:LEU:CD2	2:C:259:ASN:HD21	2.17	0.57
1:A:103:ARG:HH11	1:A:105:ARG:HH12	1.50	0.57
1:A:129:THR:O	1:A:130:LEU:HB3	2.04	0.57
1:B:27:LEU:HG	1:B:30:LEU:HD12	1.86	0.57
2:C:31:LEU:HD23	2:C:139:CYS:SG	2.44	0.57
1:A:93:GLU:O	1:A:95:GLU:N	2.37	0.57
1:B:36:GLN:O	1:B:42:LEU:HD12	2.04	0.57
1:B:111:LEU:HD12	1:B:111:LEU:N	2.20	0.57
2:D:257:LEU:HD21	2:D:286:MET:HB3	1.85	0.57
1:A:269:ARG:HD2	1:A:304:GLU:OE1	2.04	0.57
2:C:39:ARG:HH21	2:C:79:THR:CG2	2.16	0.57
2:D:2:ILE:HD11	2:D:18:ARG:NH2	2.18	0.57
2:D:279:TRP:HE3	2:D:279:TRP:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:309:GLU:O	2:D:313:LYS:HE2	2.05	0.57
1:B:137:ARG:NH1	1:B:180:CYS:SG	2.78	0.57
1:B:170:VAL:HA	1:B:178:ALA:O	2.05	0.57
2:D:299:ARG:HB3	2:D:299:ARG:CZ	2.35	0.57
1:A:53:MET:SD	1:A:230:PHE:HB3	2.45	0.57
1:B:299:GLN:OE1	1:B:301:GLU:HG2	2.05	0.57
2:C:100:LEU:C	2:C:102:GLY:H	2.13	0.57
1:B:231:ILE:O	1:B:231:ILE:HG22	2.02	0.57
2:C:304:LEU:HB3	2:C:327:LEU:HD21	1.87	0.57
2:D:278:VAL:HG12	2:D:278:VAL:O	2.05	0.57
1:B:138:LEU:CD2	1:B:182:MET:HG2	2.35	0.57
1:B:88:ILE:N	1:B:88:ILE:HD12	2.19	0.56
2:D:226:SER:HB3	2:D:332:CYS:SG	2.44	0.56
2:D:227:LYS:HD2	2:D:227:LYS:N	2.13	0.56
2:D:230:LEU:HD11	2:D:325:GLU:CG	2.35	0.56
1:B:265:GLN:O	1:B:266:ALA:C	2.48	0.56
1:B:349:ILE:N	1:B:349:ILE:HD12	2.19	0.56
2:C:22:LEU:CD1	2:C:112:VAL:HB	2.34	0.56
1:B:63:HIS:O	1:B:64:GLU:HG2	2.05	0.56
2:D:7:GLU:OE2	2:D:7:GLU:N	2.37	0.56
1:A:177:LEU:C	1:A:177:LEU:HD23	2.31	0.56
1:A:362:MET:HE2	2:C:72:SER:O	2.06	0.56
2:C:250:LEU:C	2:C:252:ARG:H	2.13	0.56
1:A:119:LEU:O	1:A:120:ASP:C	2.49	0.56
2:C:261:LYS:C	2:C:263:GLN:H	2.12	0.56
1:A:299:GLN:OE1	1:A:301:GLU:HG2	2.05	0.56
1:B:93:GLU:O	1:B:95:GLU:N	2.36	0.56
2:D:100:LEU:C	2:D:102:GLY:H	2.12	0.56
1:B:122:TRP:CE2	1:B:222:ASN:HB2	2.41	0.56
2:C:81:LEU:CD1	2:C:111:ILE:HB	2.36	0.56
2:C:115:ASN:O	2:C:116:LYS:C	2.49	0.56
2:C:215:PHE:O	2:C:219:ASP:HB2	2.06	0.56
2:C:192:TRP:HB3	2:C:201:ARG:NH1	2.20	0.55
2:C:220:ALA:HB1	2:C:229:ALA:HB2	1.87	0.55
2:C:235:GLN:O	2:C:239:GLU:HG3	2.06	0.55
2:C:4:LEU:HD21	2:C:12:GLN:HB2	1.89	0.55
2:C:263:GLN:HB3	2:C:266:HIS:HB3	1.88	0.55
2:D:31:LEU:HD23	2:D:139:CYS:SG	2.46	0.55
1:A:365:ARG:HH21	2:C:105:HIS:CE1	2.25	0.55
2:C:2:ILE:HD11	2:C:18:ARG:NH2	2.22	0.55
2:C:273:PHE:CZ	2:C:286:MET:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:GLU:HB3	1:B:217:GLN:HG2	1.88	0.55
1:B:223:ILE:CG2	1:B:236:LEU:HD21	2.36	0.55
2:C:173:CYS:CB	2:C:212:PHE:HE1	2.18	0.55
1:B:1:MET:HA	1:B:65:PRO:O	2.06	0.55
2:C:307:ARG:O	2:C:311:THR:HG23	2.07	0.55
1:A:277:LYS:HE3	2:C:62:ASN:ND2	2.22	0.55
2:D:225:LYS:HG3	2:D:227:LYS:HZ3	1.72	0.55
2:D:236:LEU:HD13	2:D:246:LEU:HD21	1.87	0.55
1:A:214:LEU:HD12	1:A:215:ARG:N	2.22	0.55
2:D:22:LEU:CD1	2:D:112:VAL:HB	2.35	0.55
1:A:129:THR:HG22	1:A:130:LEU:N	2.22	0.55
1:B:277:LYS:HE3	2:D:62:ASN:ND2	2.21	0.55
2:D:184:ALA:O	2:D:188:LEU:HD12	2.07	0.55
2:D:230:LEU:HD11	2:D:325:GLU:HG3	1.89	0.55
2:D:231:HIS:CE1	2:D:235:GLN:HE21	2.25	0.55
2:D:293:LEU:HD23	2:D:294:SER:H	1.72	0.55
2:C:314:GLN:HA	2:C:316:TYR:HE2	1.72	0.54
1:A:127:GLU:HA	1:A:216:VAL:O	2.08	0.54
2:D:272:LEU:HD12	2:D:275:LYS:CB	2.38	0.54
1:B:138:LEU:HD23	1:B:180:CYS:SG	2.47	0.54
2:C:309:GLU:HA	2:C:312:LEU:HD21	1.90	0.54
1:A:222:ASN:ND2	1:A:235:LYS:NZ	2.52	0.54
1:B:129:THR:HG22	1:B:130:LEU:N	2.21	0.54
1:B:172:THR:OG1	1:B:177:LEU:HB2	2.07	0.54
2:C:68:CYS:O	2:C:105:HIS:HE1	1.90	0.54
2:C:218:VAL:HG11	2:C:253:GLU:HG3	1.90	0.54
2:C:332:CYS:O	2:C:333:HIS:C	2.50	0.54
2:D:207:ASN:HD22	2:D:207:ASN:N	2.06	0.54
1:B:80:ARG:HE	1:B:80:ARG:C	2.16	0.54
2:D:1:MET:CB	2:D:131:ALA:O	2.50	0.54
2:D:244:VAL:HG22	2:D:312:LEU:HD22	1.87	0.54
1:A:278:PHE:CD1	1:A:278:PHE:C	2.86	0.54
2:C:11:ALA:O	2:C:13:LEU:N	2.38	0.54
2:C:212:PHE:HB3	2:C:215:PHE:CD1	2.42	0.54
2:D:251:GLN:HB2	2:D:305:LEU:HD22	1.89	0.54
2:D:272:LEU:HD12	2:D:275:LYS:HB3	1.90	0.54
1:B:2:LYS:CG	1:B:64:GLU:HB2	2.35	0.54
2:C:214:PRO:HB3	2:C:246:LEU:HD23	1.87	0.54
1:A:197:ARG:O	1:A:201:ILE:HG12	2.08	0.54
1:B:50:GLU:OE2	1:B:198:LYS:HD2	2.08	0.54
2:D:198:THR:OG1	2:D:201:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:52:THR:HG23	2:C:81:LEU:HD23	1.89	0.54
1:A:135:MET:O	1:A:135:MET:SD	2.66	0.54
1:A:278:PHE:CD1	1:A:278:PHE:O	2.61	0.54
1:B:194:ILE:HG22	1:B:237:VAL:HB	1.90	0.54
1:A:170:VAL:HG22	1:A:241:PHE:CE2	2.43	0.53
1:A:362:MET:HE3	2:C:71:MET:CB	2.32	0.53
1:B:226:HIS:N	1:B:226:HIS:CD2	2.75	0.53
1:B:222:ASN:OD1	1:B:235:LYS:NZ	2.40	0.53
2:C:225:LYS:HE2	2:C:228:ARG:CG	2.38	0.53
2:D:293:LEU:HD13	2:D:298:LEU:HD13	1.90	0.53
2:D:307:ARG:O	2:D:311:THR:OG1	2.25	0.53
1:A:130:LEU:HD21	1:A:135:MET:CB	2.38	0.53
2:C:184:ALA:O	2:C:188:LEU:HD12	2.08	0.53
2:C:325:GLU:N	2:C:325:GLU:OE1	2.42	0.53
2:D:52:THR:HG23	2:D:81:LEU:HD23	1.91	0.53
2:D:254:LEU:HD11	2:D:298:LEU:HD12	1.89	0.53
1:A:177:LEU:HD21	1:A:179:VAL:CG2	2.35	0.53
1:B:139:ILE:O	1:B:143:GLN:HB2	2.08	0.53
1:A:256:LEU:C	1:A:256:LEU:HD12	2.33	0.53
1:B:293:THR:HB	1:B:303:GLU:CB	2.39	0.53
2:C:166:ALA:HB2	2:C:199:LEU:HA	1.91	0.53
2:D:221:LEU:O	2:D:223:MET:N	2.30	0.53
2:D:260:LEU:HD13	2:D:290:LEU:HD11	1.91	0.53
1:A:135:MET:CE	1:A:160:PHE:HE2	2.22	0.53
2:C:192:TRP:CD2	2:C:201:ARG:HD3	2.43	0.53
1:A:129:THR:HG22	1:A:130:LEU:H	1.74	0.53
1:A:170:VAL:HG22	1:A:241:PHE:HE2	1.74	0.53
1:A:256:LEU:CD1	1:A:308:VAL:HG21	2.38	0.53
1:A:268:ALA:O	1:A:271:ALA:HB3	2.07	0.53
1:A:278:PHE:O	1:A:278:PHE:HD1	1.91	0.53
1:A:319:PHE:HZ	1:A:347:VAL:HG21	1.74	0.53
2:D:115:ASN:O	2:D:116:LYS:C	2.52	0.53
2:D:207:ASN:C	2:D:209:ALA:H	2.17	0.53
2:D:305:LEU:HD23	2:D:305:LEU:O	2.08	0.53
1:A:2:LYS:CG	1:A:64:GLU:HB2	2.33	0.53
1:A:344:VAL:HA	2:C:71:MET:HE1	1.90	0.53
2:D:260:LEU:HB3	2:D:290:LEU:CD1	2.39	0.53
1:B:319:PHE:HZ	1:B:347:VAL:HG21	1.73	0.52
2:C:225:LYS:CG	2:C:228:ARG:HG3	2.39	0.52
2:C:256:LEU:HA	2:C:259:ASN:HD22	1.72	0.52
2:D:312:LEU:O	2:D:316:TYR:CD2	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:THR:HB	1:A:303:GLU:CB	2.39	0.52
1:A:308:VAL:CG2	1:A:309:THR:H	2.21	0.52
1:A:308:VAL:CG2	1:A:309:THR:N	2.72	0.52
1:B:271:ALA:HB2	1:B:321:VAL:HG11	1.91	0.52
2:C:100:LEU:C	2:C:102:GLY:N	2.65	0.52
2:D:214:PRO:HB3	2:D:246:LEU:HD23	1.91	0.52
1:A:1:MET:HA	1:A:65:PRO:O	2.08	0.52
1:A:170:VAL:CG2	1:A:241:PHE:HE2	2.23	0.52
1:A:197:ARG:NH1	1:A:197:ARG:HB3	2.24	0.52
1:B:1:MET:HB3	1:B:66:GLY:CA	2.28	0.52
1:B:278:PHE:CD1	1:B:278:PHE:C	2.86	0.52
2:C:245:ILE:C	2:C:245:ILE:HD13	2.34	0.52
2:C:277:ARG:C	2:C:278:VAL:HA	2.31	0.52
1:A:80:ARG:C	1:A:80:ARG:HE	2.17	0.52
1:A:310:TYR:CG	1:A:311:SER:N	2.78	0.52
1:B:258:ALA:HB3	1:B:263:LEU:HD11	1.92	0.52
1:B:308:VAL:CG2	1:B:309:THR:N	2.71	0.52
2:C:243:PRO:C	2:C:245:ILE:N	2.67	0.52
2:D:300:GLN:O	2:D:303:GLN:HB2	2.09	0.52
1:B:196:PRO:HG3	1:B:237:VAL:HG23	1.92	0.52
1:B:260:CYS:O	1:B:264:LYS:HG3	2.09	0.52
2:C:92:ALA:O	2:C:95:GLU:HB2	2.09	0.52
2:D:296:THR:HB	2:D:297:GLN:NE2	2.24	0.52
1:A:337:ARG:HG2	1:A:339:MET:HE2	1.91	0.52
1:B:298:GLU:O	1:B:299:GLN:HB2	2.09	0.52
2:C:293:LEU:HD23	2:C:297:GLN:OE1	2.09	0.52
1:B:256:LEU:HD12	1:B:256:LEU:C	2.35	0.52
2:D:56:ASP:HB2	2:D:57:PRO:CD	2.38	0.52
2:D:100:LEU:C	2:D:102:GLY:N	2.67	0.52
1:B:218:ILE:N	1:B:218:ILE:HD12	2.25	0.52
1:B:232:PHE:CZ	1:B:234:SER:HB2	2.45	0.52
1:A:246:ARG:HH11	1:A:246:ARG:CB	2.16	0.52
1:A:258:ALA:HB3	1:A:263:LEU:HD11	1.92	0.52
1:B:173:ASP:OD1	1:B:176:ARG:HD2	2.10	0.52
1:B:218:ILE:HD12	1:B:218:ILE:H	1.74	0.52
2:C:90:ASN:HD22	2:C:91:ALA:H	1.55	0.52
1:A:197:ARG:HB2	1:A:198:LYS:HE2	1.91	0.51
1:B:268:ALA:O	1:B:271:ALA:HB3	2.10	0.51
2:C:263:GLN:CB	2:C:266:HIS:HB3	2.40	0.51
2:C:314:GLN:HA	2:C:316:TYR:CE2	2.45	0.51
1:B:256:LEU:CD1	1:B:308:VAL:HG21	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:ARG:O	2:D:231:HIS:HB3	2.11	0.51
1:A:77:ASP:O	1:A:81:GLY:N	2.42	0.51
2:D:203:GLU:C	2:D:205:ALA:N	2.68	0.51
2:D:289:ALA:C	2:D:291:ASN:H	2.17	0.51
2:C:255:LEU:HD23	2:C:255:LEU:O	2.09	0.51
2:D:158:LEU:O	2:D:160:LEU:HD13	2.09	0.51
2:D:260:LEU:HB3	2:D:290:LEU:HD13	1.92	0.51
1:A:277:LYS:HE3	2:C:62:ASN:HD21	1.75	0.51
1:A:341:THR:HG22	1:A:342:ASP:HB2	1.93	0.51
2:D:223:MET:HE2	2:D:289:ALA:CA	2.33	0.51
1:B:204:MET:HE3	1:B:204:MET:O	2.11	0.51
1:B:362:MET:HG2	2:D:73:LEU:HG	1.93	0.51
2:D:166:ALA:HB2	2:D:199:LEU:HA	1.91	0.51
1:A:184:ILE:HG13	1:A:185:GLY:N	2.26	0.51
1:B:97:MET:HB3	1:B:108:LEU:HB2	1.92	0.51
2:C:247:LEU:HD22	2:C:305:LEU:HG	1.93	0.51
2:D:293:LEU:CD2	2:D:298:LEU:HB2	2.41	0.51
1:A:61:GLN:HB3	1:A:62:PRO:HD2	1.93	0.51
1:B:77:ASP:O	1:B:81:GLY:N	2.43	0.51
2:C:26:ASN:N	2:C:140:GLN:HE22	2.07	0.51
1:A:177:LEU:CD2	1:A:179:VAL:HG23	2.38	0.51
1:A:331:LEU:C	1:A:333:CYS:H	2.19	0.51
1:A:362:MET:CE	2:C:71:MET:HB3	2.33	0.51
1:B:206:MET:HE2	1:B:227:VAL:CG2	2.41	0.51
1:B:305:ILE:CG2	1:B:306:LEU:N	2.74	0.51
1:B:308:VAL:CG2	1:B:309:THR:H	2.21	0.51
2:C:256:LEU:O	2:C:260:LEU:HG	2.11	0.51
2:D:92:ALA:O	2:D:95:GLU:HB2	2.11	0.51
2:D:150:TRP:CZ2	2:D:178:LEU:HD12	2.46	0.51
2:D:217:TRP:CE2	2:D:221:LEU:HD12	2.45	0.51
1:A:138:LEU:HD21	1:A:182:MET:HG2	1.93	0.51
2:C:97:LEU:HD23	2:C:126:TRP:CD2	2.46	0.51
2:C:158:LEU:O	2:C:160:LEU:HD13	2.11	0.51
1:A:14:LEU:CD2	1:A:76:PHE:HA	2.41	0.50
1:B:51:MET:HB2	1:B:232:PHE:CE1	2.44	0.50
1:B:61:GLN:HB3	1:B:62:PRO:HD2	1.92	0.50
1:B:278:PHE:CD1	1:B:278:PHE:O	2.64	0.50
2:C:11:ALA:C	2:C:13:LEU:N	2.69	0.50
2:D:97:LEU:HD23	2:D:126:TRP:CD2	2.46	0.50
1:A:70:VAL:HG21	1:A:75:PHE:CD2	2.46	0.50
1:B:14:LEU:CD2	1:B:76:PHE:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:HD21	1:B:135:MET:HG2	1.93	0.50
2:C:245:ILE:HG23	2:C:246:LEU:N	2.25	0.50
2:D:55:ILE:HD12	2:D:61:TRP:CH2	2.46	0.50
2:D:81:LEU:CD1	2:D:111:ILE:HB	2.42	0.50
2:D:313:LYS:HA	2:D:316:TYR:CE2	2.46	0.50
2:C:91:ALA:O	2:C:95:GLU:OE1	2.30	0.50
1:A:8:GLU:C	1:A:10:LEU:H	2.19	0.50
1:A:271:ALA:HB2	1:A:321:VAL:HG11	1.93	0.50
1:A:298:GLU:O	1:A:299:GLN:HB2	2.09	0.50
1:B:83:PRO:HG2	1:B:86:ALA:CB	2.41	0.50
2:C:296:THR:HA	2:C:299:ARG:NH1	2.26	0.50
2:D:91:ALA:O	2:D:95:GLU:OE1	2.30	0.50
1:B:278:PHE:O	1:B:278:PHE:HD1	1.95	0.50
1:B:310:TYR:CG	1:B:311:SER:N	2.80	0.50
1:B:341:THR:HG22	1:B:342:ASP:N	2.26	0.50
1:A:16:GLN:NE2	1:A:230:PHE:CD1	2.74	0.50
1:A:122:TRP:CD1	1:A:122:TRP:N	2.79	0.50
2:C:270:ARG:O	2:C:274:ASP:CG	2.54	0.50
2:D:44:ALA:O	2:D:45:GLN:HG3	2.11	0.50
2:D:126:TRP:CG	2:D:127:PHE:N	2.80	0.50
2:D:254:LEU:O	2:D:258:VAL:HG23	2.11	0.50
2:D:313:LYS:C	2:D:316:TYR:CE2	2.90	0.50
1:A:281:VAL:HG12	1:A:282:ARG:N	2.27	0.50
1:B:60:VAL:HG23	1:B:61:GLN:N	2.27	0.50
1:B:147:ALA:HB2	1:B:173:ASP:HA	1.94	0.50
1:B:281:VAL:HG12	1:B:282:ARG:N	2.27	0.50
2:C:221:LEU:HD12	2:C:250:LEU:HD13	1.93	0.50
2:D:313:LYS:O	2:D:316:TYR:CE2	2.64	0.50
1:A:83:PRO:HG2	1:A:86:ALA:CB	2.41	0.50
2:C:31:LEU:HD23	2:C:139:CYS:CB	2.42	0.50
2:D:100:LEU:C	2:D:100:LEU:HD23	2.37	0.49
2:D:215:PHE:CE2	2:D:249:THR:HG23	2.47	0.49
2:D:253:GLU:HB3	2:D:286:MET:SD	2.52	0.49
1:A:197:ARG:HB3	1:A:197:ARG:CZ	2.42	0.49
1:B:261:ASP:OD2	1:B:262:LEU:N	2.45	0.49
2:C:126:TRP:CG	2:C:127:PHE:N	2.80	0.49
1:A:97:MET:HB3	1:A:108:LEU:HB2	1.94	0.49
1:A:266:ALA:HB1	1:A:292:ILE:CG2	2.28	0.49
1:B:27:LEU:HD12	1:B:29:ILE:HG22	1.94	0.49
2:C:100:LEU:C	2:C:100:LEU:HD23	2.37	0.49
2:C:150:TRP:CZ2	2:C:178:LEU:HD12	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:MET:HE2	1:B:135:MET:HA	1.94	0.49
1:A:168:ARG:HE	1:A:181:SER:HG	1.57	0.49
1:A:323:TYR:O	1:A:327:VAL:HG23	2.13	0.49
2:C:55:ILE:HD12	2:C:61:TRP:CH2	2.46	0.49
2:D:278:VAL:CG1	2:D:282:ARG:HH11	2.25	0.49
1:A:20:PRO:HB3	1:A:202:GLU:HG2	1.95	0.49
1:A:60:VAL:HG23	1:A:61:GLN:N	2.26	0.49
1:A:155:LEU:C	1:A:157:GLY:H	2.21	0.49
1:A:184:ILE:HD12	1:A:188:LEU:HD11	1.95	0.49
1:B:70:VAL:HG21	1:B:75:PHE:CD2	2.48	0.49
2:D:68:CYS:O	2:D:105:HIS:HE1	1.95	0.49
1:B:295:ASN:CG	1:B:297:PRO:HD3	2.38	0.49
1:B:331:LEU:C	1:B:333:CYS:H	2.21	0.49
1:B:362:MET:HE3	2:D:71:MET:HB3	1.93	0.49
2:C:147:LEU:HB3	2:C:148:PRO:HD3	1.95	0.49
2:D:217:TRP:NE1	2:D:221:LEU:HD12	2.28	0.49
2:D:279:TRP:O	2:D:282:ARG:N	2.46	0.49
1:A:269:ARG:HH11	1:A:269:ARG:HG2	1.78	0.49
1:A:288:ASN:H	1:A:310:TYR:HB3	1.77	0.49
2:D:11:ALA:O	2:D:13:LEU:N	2.44	0.49
1:A:70:VAL:HA	1:A:110:THR:HG22	1.95	0.49
1:A:162:THR:O	1:A:190:SER:HA	2.13	0.49
1:B:203:LEU:O	1:B:207:LEU:HG	2.13	0.49
2:C:231:HIS:C	2:C:231:HIS:HD2	2.18	0.49
2:D:297:GLN:O	2:D:299:ARG:N	2.46	0.49
1:B:10:LEU:C	1:B:13:PRO:HD2	2.38	0.49
2:C:27:ASP:OD1	2:C:27:ASP:C	2.55	0.49
2:C:222:LEU:HD12	2:C:285:MET:CE	2.42	0.49
2:C:309:GLU:HA	2:C:312:LEU:CD2	2.43	0.49
2:D:147:LEU:HB3	2:D:148:PRO:HD3	1.94	0.49
2:D:322:ALA:O	2:D:325:GLU:HB3	2.12	0.49
1:A:34:LEU:HD11	1:A:113:ALA:HB1	1.95	0.48
2:C:7:GLU:OE2	2:C:7:GLU:N	2.40	0.48
2:C:31:LEU:HD23	2:C:139:CYS:HB2	1.95	0.48
2:D:225:LYS:HD3	2:D:228:ARG:NH2	2.26	0.48
1:A:130:LEU:CD2	1:A:135:MET:HB2	2.40	0.48
1:A:295:ASN:CG	1:A:297:PRO:HD3	2.38	0.48
1:B:93:GLU:OE1	1:B:98:LEU:HD21	2.13	0.48
2:D:48:GLU:HG2	2:D:76:SER:CB	2.43	0.48
2:D:254:LEU:HD21	2:D:301:ALA:CB	2.42	0.48
2:D:273:PHE:HB3	2:D:279:TRP:CD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:C	1:A:11:LEU:HD23	2.39	0.48
1:A:130:LEU:HD13	1:A:130:LEU:O	2.13	0.48
1:A:184:ILE:HD11	1:A:188:LEU:HG	1.95	0.48
1:B:8:GLU:C	1:B:10:LEU:H	2.20	0.48
1:B:70:VAL:HG11	1:B:97:MET:SD	2.53	0.48
2:D:156:LYS:C	2:D:158:LEU:H	2.20	0.48
2:D:207:ASN:N	2:D:207:ASN:ND2	2.58	0.48
1:A:20:PRO:HD3	1:A:202:GLU:OE2	2.12	0.48
1:A:261:ASP:OD2	1:A:262:LEU:N	2.47	0.48
1:B:70:VAL:HA	1:B:110:THR:HG22	1.96	0.48
1:B:147:ALA:HB1	1:B:150:ASP:HB2	1.95	0.48
2:C:64:ILE:O	2:C:67:LEU:HB3	2.13	0.48
2:C:243:PRO:O	2:C:245:ILE:N	2.46	0.48
2:D:206:VAL:O	2:D:209:ALA:HB3	2.14	0.48
2:D:221:LEU:O	2:D:221:LEU:CD2	2.58	0.48
2:D:304:LEU:CB	2:D:307:ARG:HD2	2.41	0.48
2:D:330:LEU:HD13	2:D:330:LEU:C	2.38	0.48
1:B:32:ASN:HB3	1:B:69:THR:CG2	2.43	0.48
2:D:142:PRO:HD2	2:D:178:LEU:HD21	1.95	0.48
1:A:194:ILE:HD11	1:A:241:PHE:HB2	1.95	0.48
1:B:246:ARG:HH11	1:B:246:ARG:CB	2.16	0.48
1:B:197:ARG:CG	1:B:198:LYS:N	2.75	0.48
2:C:142:PRO:HD2	2:C:178:LEU:HD21	1.96	0.48
2:C:225:LYS:O	2:C:225:LYS:HG2	2.14	0.48
1:A:29:ILE:HD12	1:A:69:THR:HG21	1.96	0.48
1:A:210:GLY:C	1:A:212:ASN:H	2.22	0.48
1:B:265:GLN:NE2	1:B:269:ARG:NH2	2.62	0.48
2:C:156:LYS:C	2:C:158:LEU:H	2.20	0.48
1:B:29:ILE:HD12	1:B:69:THR:HG21	1.95	0.48
1:B:224:ARG:HD2	1:B:226:HIS:NE2	2.28	0.48
2:D:78:GLN:HG3	2:D:108:LEU:HD13	1.95	0.48
2:D:304:LEU:HA	2:D:307:ARG:HB2	1.96	0.48
1:A:32:ASN:HB3	1:A:69:THR:CG2	2.44	0.48
1:B:11:LEU:C	1:B:11:LEU:HD23	2.39	0.48
1:B:162:THR:O	1:B:163:GLU:HB3	2.14	0.48
2:D:271:ALA:C	2:D:273:PHE:N	2.72	0.48
1:A:10:LEU:C	1:A:13:PRO:HD2	2.39	0.47
1:A:11:LEU:HD23	1:A:11:LEU:O	2.13	0.47
2:D:207:ASN:ND2	2:D:207:ASN:H	2.12	0.47
1:A:170:VAL:HB	1:A:179:VAL:HG22	1.96	0.47
1:A:288:ASN:N	1:A:288:ASN:ND2	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ILE:HG22	1:A:350:GLU:N	2.29	0.47
1:B:337:ARG:HG2	1:B:339:MET:HE2	1.96	0.47
2:C:56:ASP:HB2	2:C:57:PRO:CD	2.41	0.47
1:A:305:ILE:CG2	1:A:306:LEU:N	2.76	0.47
1:A:316:GLU:O	1:A:316:GLU:HG3	2.14	0.47
1:B:11:LEU:HD23	1:B:11:LEU:O	2.14	0.47
1:B:27:LEU:HD12	1:B:29:ILE:CG2	2.45	0.47
2:C:177:ASN:HB2	2:C:241:SER:HA	1.97	0.47
2:C:257:LEU:O	2:C:290:LEU:HD21	2.14	0.47
2:C:277:ARG:O	2:C:278:VAL:HA	2.15	0.47
1:B:135:MET:HG3	1:B:214:LEU:HD23	1.94	0.47
2:C:31:LEU:CD1	2:C:113:ARG:HE	2.27	0.47
2:C:305:LEU:HB2	2:C:327:LEU:HD11	1.97	0.47
2:D:254:LEU:CD1	2:D:298:LEU:HD12	2.44	0.47
1:B:288:ASN:H	1:B:310:TYR:HB3	1.78	0.47
1:B:341:THR:HG22	1:B:342:ASP:HB2	1.97	0.47
1:A:32:ASN:ND2	1:A:70:VAL:C	2.73	0.47
1:B:214:LEU:HD12	1:B:215:ARG:N	2.29	0.47
2:C:236:LEU:O	2:C:241:SER:HB3	2.15	0.47
2:C:250:LEU:C	2:C:252:ARG:N	2.72	0.47
1:A:363:PRO:HG2	2:C:71:MET:CE	2.41	0.47
2:C:101:THR:CG2	2:C:126:TRP:HB2	2.45	0.47
2:D:231:HIS:HE1	2:D:235:GLN:HE21	1.62	0.47
2:D:306:THR:HA	2:D:309:GLU:HG2	1.95	0.47
1:B:269:ARG:HG2	1:B:269:ARG:HH11	1.80	0.47
2:C:78:GLN:HG3	2:C:108:LEU:HD13	1.96	0.47
2:D:95:GLU:O	2:D:98:LEU:HB3	2.15	0.47
2:D:283:ARG:O	2:D:283:ARG:HG2	2.15	0.47
1:A:126:VAL:HG22	1:A:127:GLU:N	2.30	0.47
1:A:304:GLU:C	1:A:305:ILE:HD12	2.40	0.47
2:C:48:GLU:HG2	2:C:76:SER:CB	2.44	0.47
2:D:31:LEU:HD23	2:D:139:CYS:CB	2.45	0.47
1:A:44:LEU:HD12	1:A:44:LEU:N	2.30	0.46
1:A:219:GLY:O	1:A:220:SER:C	2.58	0.46
1:B:34:LEU:HD11	1:B:113:ALA:HB1	1.96	0.46
1:B:256:LEU:HD12	1:B:257:GLU:N	2.30	0.46
2:C:273:PHE:CE2	2:C:283:ARG:HA	2.50	0.46
2:D:101:THR:CG2	2:D:126:TRP:HB2	2.45	0.46
2:D:117:LEU:HD23	2:D:117:LEU:HA	1.75	0.46
2:D:214:PRO:CB	2:D:246:LEU:HD23	2.45	0.46
1:A:256:LEU:HD12	1:A:257:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLN:NE2	1:A:269:ARG:NH2	2.63	0.46
1:B:134:THR:C	1:B:136:LYS:N	2.74	0.46
1:B:253:ASP:OD2	1:B:254:LYS:HG3	2.15	0.46
1:B:283:LEU:O	1:B:316:GLU:HA	2.15	0.46
1:B:338:MET:HE2	1:B:349:ILE:HG13	1.95	0.46
2:C:308:THR:O	2:C:312:LEU:HD22	2.16	0.46
2:D:54:SER:HA	2:D:83:LEU:HB2	1.98	0.46
2:D:64:ILE:O	2:D:67:LEU:HB3	2.15	0.46
2:D:309:GLU:O	2:D:313:LYS:HG2	2.15	0.46
1:A:253:ASP:OD2	1:A:254:LYS:HG3	2.15	0.46
2:C:44:ALA:O	2:C:45:GLN:HG3	2.15	0.46
2:D:278:VAL:CG1	2:D:282:ARG:NH1	2.78	0.46
1:B:323:TYR:O	1:B:327:VAL:HG23	2.16	0.46
2:C:205:ALA:O	2:C:209:ALA:HB3	2.16	0.46
2:C:322:ALA:C	2:C:324:LEU:H	2.23	0.46
2:D:218:VAL:C	2:D:220:ALA:H	2.23	0.46
1:B:122:TRP:HZ3	1:B:219:GLY:HA3	1.79	0.46
1:B:316:GLU:HG3	1:B:316:GLU:O	2.15	0.46
2:D:271:ALA:C	2:D:273:PHE:H	2.22	0.46
2:C:90:ASN:CG	2:C:91:ALA:H	2.22	0.46
2:C:95:GLU:O	2:C:98:LEU:HB3	2.16	0.46
2:C:119:LYS:H	2:C:119:LYS:HG2	1.53	0.46
2:C:252:ARG:O	2:C:253:GLU:C	2.59	0.46
2:D:9:LEU:HG	2:D:13:LEU:HD22	1.97	0.46
2:D:263:GLN:C	2:D:265:ALA:H	2.23	0.46
2:D:300:GLN:HG3	2:D:303:GLN:NE2	2.31	0.46
1:A:96:ARG:NH1	1:A:107:SER:OG	2.49	0.46
2:D:198:THR:O	2:D:202:VAL:HG23	2.16	0.46
1:A:4:THR:HG22	1:A:61:GLN:NE2	2.31	0.46
1:A:283:LEU:O	1:A:316:GLU:HA	2.16	0.46
1:B:206:MET:O	1:B:207:LEU:C	2.59	0.46
1:B:212:ASN:O	1:B:214:LEU:N	2.49	0.46
2:D:27:ASP:C	2:D:27:ASP:OD1	2.59	0.46
2:D:217:TRP:HA	2:D:232:ILE:CD1	2.46	0.46
1:A:168:ARG:NE	1:A:181:SER:OG	2.46	0.46
1:B:82:LEU:HD13	1:B:101:SER:HB2	1.97	0.46
1:B:295:ASN:ND2	1:B:297:PRO:HD3	2.31	0.46
2:C:105:HIS:CD2	2:C:106:ASP:H	2.34	0.46
2:D:48:GLU:HG2	2:D:76:SER:HB2	1.98	0.46
1:A:227:VAL:O	1:A:227:VAL:HG12	2.15	0.45
1:A:338:MET:HE2	1:A:349:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:97:LEU:HD23	2:C:126:TRP:CE2	2.51	0.45
2:D:150:TRP:CZ3	2:D:178:LEU:HD12	2.51	0.45
2:D:292:ARG:HB2	2:D:292:ARG:CZ	2.44	0.45
1:A:349:ILE:O	1:A:350:GLU:HB3	2.16	0.45
1:B:134:THR:C	1:B:136:LYS:H	2.23	0.45
1:B:143:GLN:HG2	1:B:143:GLN:O	2.17	0.45
2:C:54:SER:HA	2:C:83:LEU:HB2	1.98	0.45
1:B:32:ASN:ND2	1:B:70:VAL:C	2.74	0.45
2:C:39:ARG:NH2	2:C:79:THR:HG22	2.25	0.45
2:C:226:SER:O	2:C:229:ALA:HB3	2.17	0.45
2:D:202:VAL:O	2:D:205:ALA:HB3	2.17	0.45
2:D:311:THR:HG22	2:D:315:ASP:CB	2.35	0.45
1:A:82:LEU:HD13	1:A:101:SER:HB2	1.97	0.45
1:A:152:ARG:NH2	2:C:49:GLU:HG3	2.32	0.45
1:B:162:THR:O	1:B:190:SER:HA	2.16	0.45
1:B:349:ILE:O	1:B:350:GLU:HB3	2.16	0.45
2:C:126:TRP:O	2:C:129:ALA:HB3	2.16	0.45
2:C:192:TRP:C	2:C:194:ASP:N	2.74	0.45
2:D:31:LEU:HD23	2:D:139:CYS:HB2	1.98	0.45
2:D:170:LEU:HG	2:D:202:VAL:HG11	1.98	0.45
1:A:78:ILE:O	1:A:82:LEU:HG	2.16	0.45
1:A:135:MET:HE3	1:A:160:PHE:HE2	1.82	0.45
1:A:295:ASN:ND2	1:A:297:PRO:HD3	2.32	0.45
1:B:122:TRP:CZ3	1:B:219:GLY:HA3	2.52	0.45
1:B:194:ILE:HG21	1:B:237:VAL:HB	1.97	0.45
1:B:247:VAL:O	1:B:248:LEU:C	2.60	0.45
2:D:26:ASN:N	2:D:140:GLN:HE22	2.10	0.45
2:D:97:LEU:HD23	2:D:126:TRP:CE2	2.51	0.45
1:A:93:GLU:OE1	1:A:98:LEU:HD21	2.16	0.45
1:B:349:ILE:HG22	1:B:350:GLU:N	2.31	0.45
2:C:9:LEU:HG	2:C:13:LEU:HD22	1.99	0.45
2:C:117:LEU:O	2:C:118:SER:C	2.60	0.45
2:D:90:ASN:CG	2:D:91:ALA:H	2.24	0.45
2:D:126:TRP:O	2:D:129:ALA:HB3	2.16	0.45
1:A:122:TRP:CD1	1:A:122:TRP:H	2.33	0.45
2:D:106:ASP:C	2:D:108:LEU:H	2.25	0.45
2:D:221:LEU:HD21	2:D:331:LEU:HB2	1.99	0.45
1:B:218:ILE:CG2	1:B:219:GLY:N	2.76	0.45
2:C:68:CYS:O	2:C:105:HIS:CE1	2.69	0.45
2:C:255:LEU:HD23	2:C:259:ASN:ND2	2.32	0.45
2:D:259:ASN:C	2:D:261:LYS:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HG11	1:A:97:MET:SD	2.57	0.45
1:A:262:LEU:HD12	1:A:262:LEU:HA	1.82	0.45
1:B:135:MET:HE3	1:B:167:LEU:HD21	1.98	0.45
2:C:141:THR:C	2:C:142:PRO:O	2.53	0.45
2:C:214:PRO:HB3	2:C:246:LEU:HD22	1.98	0.45
2:C:283:ARG:O	2:C:287:GLY:N	2.48	0.45
2:D:31:LEU:CD1	2:D:113:ARG:HE	2.30	0.45
2:D:67:LEU:HD11	2:D:78:GLN:NE2	2.32	0.45
2:D:270:ARG:HA	2:D:273:PHE:CE1	2.52	0.45
2:D:293:LEU:HD22	2:D:298:LEU:HB2	1.99	0.45
1:A:27:LEU:HD12	1:A:29:ILE:CG2	2.47	0.44
1:B:78:ILE:O	1:B:82:LEU:HG	2.17	0.44
2:C:31:LEU:HD13	2:C:113:ARG:CG	2.47	0.44
2:C:171:CYS:O	2:C:175:GLU:HB2	2.17	0.44
2:C:192:TRP:CG	2:C:201:ARG:HH11	2.34	0.44
2:C:222:LEU:C	2:C:224:GLY:H	2.24	0.44
2:C:249:THR:OG1	2:C:250:LEU:N	2.49	0.44
2:D:119:LYS:H	2:D:119:LYS:HG2	1.43	0.44
1:A:70:VAL:HG23	1:A:71:PRO:O	2.18	0.44
1:A:267:PHE:HZ	1:A:283:LEU:HD11	1.81	0.44
1:A:349:ILE:N	1:A:349:ILE:CD1	2.80	0.44
1:B:44:LEU:N	1:B:44:LEU:HD12	2.32	0.44
2:C:150:TRP:CZ3	2:C:178:LEU:HD12	2.52	0.44
2:D:4:LEU:HG	2:D:8:GLN:HB2	1.99	0.44
1:A:271:ALA:O	1:A:274:SER:HB3	2.17	0.44
1:A:279:ARG:HD2	1:A:297:PRO:CG	2.44	0.44
1:B:106:PHE:CD1	1:B:106:PHE:N	2.86	0.44
1:B:214:LEU:HD13	1:B:225:ALA:HB1	1.94	0.44
1:B:224:ARG:HB2	1:B:232:PHE:O	2.17	0.44
2:D:205:ALA:O	2:D:209:ALA:HB2	2.17	0.44
1:B:49:LEU:HD21	1:B:117:PRO:HB2	1.98	0.44
1:B:279:ARG:HD2	1:B:297:PRO:CG	2.42	0.44
2:C:295:GLN:HA	2:C:298:LEU:HB2	1.99	0.44
1:A:111:LEU:HD12	1:A:111:LEU:H	1.82	0.44
1:A:177:LEU:HD23	1:A:178:ALA:N	2.33	0.44
1:B:18:SER:HA	1:B:21:LEU:HG	1.99	0.44
2:C:55:ILE:HD11	2:C:82:LEU:HG	1.99	0.44
2:C:261:LYS:C	2:C:263:GLN:N	2.75	0.44
1:A:52:GLU:O	1:A:52:GLU:HG3	2.17	0.44
1:A:95:GLU:O	1:A:96:ARG:HD3	2.18	0.44
1:A:106:PHE:CD1	1:A:106:PHE:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LEU:C	1:B:21:LEU:HD12	2.43	0.44
1:B:304:GLU:C	1:B:305:ILE:HD12	2.43	0.44
1:B:305:ILE:HG22	1:B:306:LEU:N	2.33	0.44
2:C:143:GLU:O	2:C:147:LEU:N	2.50	0.44
2:D:35:GLN:NE2	2:D:81:LEU:HD22	2.32	0.44
2:D:171:CYS:O	2:D:175:GLU:HB2	2.18	0.44
1:B:52:GLU:HG3	1:B:52:GLU:O	2.17	0.44
1:B:78:ILE:HG22	1:B:79:CYS:N	2.32	0.44
1:B:158:MET:SD	1:B:169:THR:HG21	2.57	0.44
1:B:271:ALA:O	1:B:274:SER:HB3	2.17	0.44
2:D:31:LEU:HD13	2:D:113:ARG:CG	2.48	0.44
2:D:303:GLN:O	2:D:307:ARG:N	2.51	0.44
1:B:223:ILE:CG1	1:B:224:ARG:N	2.81	0.44
2:C:36:ASP:O	2:C:37:ALA:C	2.61	0.44
2:D:199:LEU:HB3	2:D:200:PRO:CD	2.45	0.44
1:B:122:TRP:CD1	1:B:122:TRP:N	2.67	0.44
2:C:199:LEU:HB3	2:C:200:PRO:CD	2.45	0.44
2:C:247:LEU:HD21	2:C:324:LEU:HD21	2.00	0.44
1:A:42:LEU:HB2	1:A:59:LEU:HD11	2.00	0.43
1:A:78:ILE:HG22	1:A:79:CYS:N	2.32	0.43
2:C:106:ASP:C	2:C:108:LEU:H	2.26	0.43
1:A:49:LEU:HD21	1:A:117:PRO:HB2	1.99	0.43
1:A:51:MET:HB2	1:A:232:PHE:CE1	2.53	0.43
1:A:135:MET:HG3	1:A:214:LEU:HD23	2.00	0.43
2:C:247:LEU:HD13	2:C:309:GLU:HB3	1.98	0.43
2:D:55:ILE:HD11	2:D:82:LEU:HG	2.00	0.43
2:D:297:GLN:O	2:D:298:LEU:C	2.60	0.43
1:A:11:LEU:O	1:A:15:GLN:HB2	2.19	0.43
1:A:214:LEU:CD1	1:A:225:ALA:HB1	2.48	0.43
1:B:70:VAL:HG23	1:B:71:PRO:O	2.19	0.43
1:B:96:ARG:NH1	1:B:107:SER:OG	2.51	0.43
2:C:326:GLY:O	2:C:330:LEU:HB2	2.19	0.43
1:A:21:LEU:HD12	1:A:21:LEU:C	2.44	0.43
1:A:27:LEU:HD12	1:A:29:ILE:HG22	1.99	0.43
1:B:87:GLU:C	1:B:88:ILE:HD12	2.43	0.43
1:B:128:PHE:CE2	1:B:218:ILE:HD11	2.48	0.43
1:B:296:ASN:HB3	1:B:299:GLN:HB3	2.01	0.43
1:B:301:GLU:HB2	1:B:302:ALA:H	1.50	0.43
2:C:48:GLU:HG2	2:C:76:SER:HB2	2.00	0.43
2:D:68:CYS:O	2:D:105:HIS:CE1	2.71	0.43
2:D:90:ASN:HB3	2:D:93:ILE:CG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:ASN:HD22	2:D:91:ALA:H	1.58	0.43
2:D:223:MET:HE1	2:D:292:ARG:CB	2.46	0.43
1:A:215:ARG:NH2	1:A:226:HIS:CE1	2.87	0.43
1:B:131:PRO:O	1:B:132:GLN:C	2.62	0.43
1:B:132:GLN:NE2	1:B:227:VAL:CG1	2.80	0.43
1:B:224:ARG:HD2	1:B:226:HIS:CD2	2.53	0.43
1:A:138:LEU:HG	1:A:182:MET:HG3	2.00	0.43
1:B:4:THR:HG22	1:B:61:GLN:NE2	2.33	0.43
2:C:153:ALA:O	2:C:154:ARG:C	2.62	0.43
2:D:236:LEU:HD13	2:D:246:LEU:CD2	2.49	0.43
1:A:4:THR:HG22	1:A:61:GLN:HE22	1.84	0.43
1:A:184:ILE:HD11	1:A:186:GLN:O	2.18	0.43
1:B:73:ARG:NH2	1:B:76:PHE:HD2	2.17	0.43
1:B:206:MET:HE2	1:B:227:VAL:HG23	2.00	0.43
1:B:208:ASP:O	1:B:208:ASP:CG	2.61	0.43
1:B:288:ASN:N	1:B:288:ASN:ND2	2.64	0.43
2:C:5:TYR:N	2:C:8:GLN:OE1	2.51	0.43
2:C:133:ARG:O	2:C:133:ARG:CG	2.65	0.43
2:D:39:ARG:NH2	2:D:79:THR:HG22	2.23	0.43
2:D:110:LEU:HG	2:D:111:ILE:N	2.34	0.43
2:D:202:VAL:O	2:D:203:GLU:C	2.60	0.43
2:D:217:TRP:HA	2:D:232:ILE:HD12	1.99	0.43
2:D:224:GLY:O	2:D:225:LYS:C	2.62	0.43
2:D:235:GLN:OE1	2:D:235:GLN:HA	2.18	0.43
1:B:3:PHE:HB2	1:B:59:LEU:HD13	2.00	0.43
2:C:289:ALA:O	2:C:290:LEU:C	2.61	0.43
1:A:51:MET:HB2	1:A:233:THR:O	2.19	0.43
1:B:155:LEU:C	1:B:157:GLY:H	2.25	0.43
1:B:244:TYR:CD1	1:B:244:TYR:C	2.96	0.43
2:D:304:LEU:CD1	2:D:327:LEU:HD22	2.34	0.43
1:A:87:GLU:C	1:A:88:ILE:HD12	2.44	0.43
2:C:138:THR:O	2:C:138:THR:HG22	2.19	0.43
2:C:272:LEU:HD12	2:C:275:LYS:HG3	2.00	0.43
1:A:18:SER:HA	1:A:21:LEU:HG	2.00	0.42
1:A:73:ARG:NH2	1:A:76:PHE:HD2	2.17	0.42
1:A:254:LYS:NZ	1:A:341:THR:O	2.47	0.42
1:A:296:ASN:HB3	1:A:299:GLN:HB3	1.99	0.42
1:B:119:LEU:O	1:B:120:ASP:C	2.62	0.42
1:B:300:GLU:OE1	1:B:300:GLU:N	2.51	0.42
2:D:159:ASN:O	2:D:160:LEU:HD12	2.18	0.42
2:D:192:TRP:C	2:D:194:ASP:N	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLU:HG3	1:B:163:GLU:O	2.19	0.42
2:C:225:LYS:CG	2:C:228:ARG:CG	2.98	0.42
2:C:235:GLN:O	2:C:237:ARG:N	2.51	0.42
2:C:298:LEU:O	2:C:302:VAL:HG23	2.19	0.42
2:D:5:TYR:O	2:D:8:GLN:N	2.52	0.42
2:D:11:ALA:C	2:D:13:LEU:N	2.72	0.42
2:D:13:LEU:HD21	2:D:38:VAL:HA	2.01	0.42
2:D:213:THR:HG21	2:D:216:HIS:ND1	2.34	0.42
1:A:130:LEU:O	1:A:131:PRO:C	2.63	0.42
1:B:95:GLU:O	1:B:96:ARG:HD3	2.20	0.42
1:B:148:HIS:ND1	1:B:149:GLN:CG	2.83	0.42
2:C:90:ASN:CG	2:C:91:ALA:N	2.78	0.42
2:C:159:ASN:O	2:C:160:LEU:HD12	2.18	0.42
2:D:296:THR:O	2:D:297:GLN:C	2.62	0.42
1:A:247:VAL:O	1:A:248:LEU:C	2.63	0.42
2:C:118:SER:O	2:C:120:ALA:N	2.53	0.42
2:C:143:GLU:O	2:C:144:GLN:C	2.63	0.42
2:C:268:PRO:O	2:C:269:LEU:C	2.62	0.42
1:A:50:GLU:OE1	1:A:198:LYS:HB2	2.19	0.42
1:A:126:VAL:HG11	1:A:218:ILE:HB	1.93	0.42
2:C:1:MET:HE2	2:C:134:SER:OG	2.19	0.42
2:D:133:ARG:O	2:D:133:ARG:CG	2.66	0.42
2:D:223:MET:HG2	2:D:331:LEU:O	2.18	0.42
1:A:51:MET:SD	1:A:232:PHE:HE1	2.43	0.42
1:A:139:ILE:O	1:A:140:GLU:C	2.62	0.42
1:A:318:GLY:H	1:A:366:LEU:HD11	1.85	0.42
1:B:148:HIS:ND1	1:B:149:GLN:HG2	2.35	0.42
1:B:170:VAL:HG23	1:B:241:PHE:CE2	2.55	0.42
2:D:141:THR:C	2:D:142:PRO:O	2.58	0.42
2:D:312:LEU:O	2:D:312:LEU:HG	2.18	0.42
1:A:103:ARG:O	1:A:105:ARG:HG2	2.20	0.42
1:A:168:ARG:O	1:A:168:ARG:CG	2.68	0.42
1:A:244:TYR:CD1	1:A:244:TYR:C	2.97	0.42
1:A:301:GLU:HB2	1:A:302:ALA:H	1.51	0.42
1:B:99:VAL:HG12	1:B:100:ARG:N	2.34	0.42
2:C:90:ASN:HD22	2:C:91:ALA:N	2.15	0.42
1:A:132:GLN:OE1	1:A:209:GLY:N	2.52	0.42
1:A:292:ILE:HD13	1:A:292:ILE:O	2.19	0.42
1:B:11:LEU:O	1:B:15:GLN:HB2	2.20	0.42
2:C:223:MET:HG3	2:C:285:MET:HG2	2.01	0.42
2:C:235:GLN:C	2:C:237:ARG:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:LEU:O	2:D:118:SER:C	2.63	0.42
2:D:203:GLU:O	2:D:207:ASN:ND2	2.52	0.42
2:D:237:ARG:HE	2:D:237:ARG:HB3	1.70	0.42
1:B:224:ARG:NH1	1:B:226:HIS:CE1	2.88	0.42
1:B:267:PHE:HZ	1:B:283:LEU:HD11	1.84	0.42
2:C:5:TYR:O	2:C:8:GLN:N	2.53	0.42
2:C:311:THR:C	2:C:313:LYS:H	2.28	0.42
2:D:297:GLN:C	2:D:299:ARG:N	2.77	0.42
1:A:69:THR:OG1	1:A:113:ALA:HA	2.20	0.42
1:A:193:VAL:HB	1:A:236:LEU:HD13	2.02	0.42
1:B:288:ASN:ND2	1:B:310:TYR:H	2.17	0.42
1:B:292:ILE:HD13	1:B:292:ILE:O	2.19	0.42
2:C:279:TRP:CE2	2:C:283:ARG:HD2	2.55	0.42
2:D:275:LYS:O	2:D:275:LYS:HD3	2.20	0.42
1:A:12:LYS:HA	1:A:12:LYS:HD3	1.76	0.41
1:A:97:MET:HA	1:A:97:MET:CE	2.50	0.41
1:A:159:LEU:C	1:A:159:LEU:HD23	2.45	0.41
1:B:256:LEU:HG	1:B:338:MET:HB3	2.01	0.41
1:B:270:ALA:O	1:B:294:ALA:HB2	2.20	0.41
2:C:56:ASP:OD2	2:C:56:ASP:C	2.63	0.41
2:C:140:GLN:NE2	2:C:140:GLN:CA	2.66	0.41
2:C:261:LYS:NZ	2:C:290:LEU:O	2.51	0.41
2:D:312:LEU:HA	2:D:316:TYR:HA	2.02	0.41
1:A:27:LEU:HG	1:A:30:LEU:CD1	2.49	0.41
1:A:206:MET:HE2	1:A:227:VAL:CG2	2.50	0.41
1:B:159:LEU:HD13	1:B:241:PHE:CD2	2.54	0.41
2:C:117:LEU:HA	2:C:117:LEU:HD23	1.77	0.41
2:D:30:LEU:HB2	2:D:139:CYS:HB3	2.01	0.41
1:A:8:GLU:C	1:A:10:LEU:N	2.78	0.41
1:A:188:LEU:HB3	1:A:189:PRO:HD2	2.02	0.41
1:A:262:LEU:HG	1:A:306:LEU:CD2	2.44	0.41
1:B:103:ARG:O	1:B:105:ARG:HG2	2.20	0.41
1:A:61:GLN:HB3	1:A:62:PRO:CD	2.51	0.41
1:A:73:ARG:HA	1:A:73:ARG:NE	2.33	0.41
1:A:137:ARG:HG3	1:A:137:ARG:HH11	1.85	0.41
1:A:300:GLU:N	1:A:300:GLU:OE1	2.53	0.41
1:B:129:THR:CG2	1:B:130:LEU:N	2.84	0.41
1:B:292:ILE:O	1:B:292:ILE:HG23	2.21	0.41
1:B:347:VAL:O	1:B:360:VAL:HA	2.20	0.41
2:C:331:LEU:HD13	2:C:331:LEU:HA	1.93	0.41
1:B:9:HIS:CD2	1:B:9:HIS:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:THR:HB	1:B:27:LEU:H	1.33	0.41
1:B:185:GLY:C	1:B:186:GLN:HG3	2.45	0.41
1:B:227:VAL:HG12	1:B:227:VAL:O	2.21	0.41
2:C:227:LYS:HD2	2:C:227:LYS:H	1.85	0.41
2:D:155:ALA:O	2:D:158:LEU:HB2	2.21	0.41
2:D:214:PRO:HB3	2:D:246:LEU:CD2	2.50	0.41
2:D:245:ILE:HD12	2:D:245:ILE:N	2.36	0.41
2:D:300:GLN:HG2	2:D:307:ARG:NH2	2.35	0.41
1:A:29:ILE:CD1	1:A:69:THR:HG21	2.51	0.41
1:A:256:LEU:HG	1:A:338:MET:HB3	2.02	0.41
1:A:272:ALA:C	1:A:274:SER:N	2.78	0.41
2:D:18:ARG:HG2	2:D:134:SER:HA	2.02	0.41
2:D:40:GLN:O	2:D:41:VAL:C	2.63	0.41
2:D:153:ALA:O	2:D:154:ARG:C	2.62	0.41
1:A:99:VAL:HG12	1:A:100:ARG:N	2.36	0.41
1:A:288:ASN:ND2	1:A:310:TYR:H	2.18	0.41
1:B:61:GLN:HB3	1:B:62:PRO:CD	2.50	0.41
1:B:159:LEU:HB3	1:B:170:VAL:HG22	2.03	0.41
1:B:212:ASN:O	1:B:213:PRO:C	2.64	0.41
2:C:27:ASP:OD1	2:C:29:LEU:N	2.51	0.41
2:C:260:LEU:HB2	2:C:290:LEU:HD11	2.02	0.41
2:D:304:LEU:HA	2:D:307:ARG:CB	2.50	0.41
1:A:64:GLU:HA	1:A:65:PRO:HD3	1.91	0.41
1:A:144:PHE:CD1	1:A:144:PHE:C	2.99	0.41
1:B:272:ALA:C	1:B:274:SER:N	2.77	0.41
2:C:4:LEU:HG	2:C:8:GLN:HB2	2.01	0.41
2:C:213:THR:O	2:C:214:PRO:C	2.63	0.41
2:D:7:GLU:H	2:D:7:GLU:CD	2.27	0.41
2:D:218:VAL:C	2:D:220:ALA:N	2.78	0.41
1:A:69:THR:HG1	1:A:113:ALA:HA	1.86	0.41
1:B:29:ILE:CD1	1:B:69:THR:HG21	2.51	0.41
1:B:188:LEU:HB3	1:B:189:PRO:HD2	2.02	0.41
2:C:2:ILE:HD11	2:C:18:ARG:CZ	2.51	0.41
2:C:192:TRP:HB3	2:C:201:ARG:HH12	1.86	0.41
2:C:207:ASN:O	2:C:208:ASP:C	2.63	0.41
2:D:299:ARG:HB3	2:D:299:ARG:HH11	1.84	0.41
2:D:304:LEU:O	2:D:307:ARG:HB2	2.21	0.41
1:A:158:MET:HE3	1:A:158:MET:HB2	1.78	0.41
1:A:292:ILE:O	1:A:292:ILE:HG23	2.22	0.41
2:C:244:VAL:HG12	2:C:244:VAL:O	2.21	0.41
2:D:138:THR:O	2:D:138:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:GLN:HB2	2:D:305:LEU:CD2	2.51	0.41
1:A:168:ARG:HB2	1:A:180:CYS:O	2.20	0.40
1:A:212:ASN:O	1:A:213:PRO:C	2.63	0.40
1:B:69:THR:OG1	1:B:113:ALA:HA	2.21	0.40
2:C:4:LEU:HD11	2:C:12:GLN:HG3	2.03	0.40
2:C:52:THR:CG2	2:C:81:LEU:HD23	2.50	0.40
2:D:220:ALA:C	2:D:222:LEU:H	2.28	0.40
1:A:213:PRO:O	1:A:214:LEU:C	2.64	0.40
1:A:305:ILE:HG22	1:A:306:LEU:N	2.36	0.40
1:A:322:SER:O	1:A:323:TYR:C	2.63	0.40
1:B:135:MET:HE1	1:B:160:PHE:CE2	2.52	0.40
1:B:338:MET:HE3	1:B:338:MET:HB2	1.99	0.40
2:C:7:GLU:H	2:C:7:GLU:CD	2.29	0.40
2:C:156:LYS:C	2:C:158:LEU:N	2.80	0.40
2:C:194:ASP:OD1	2:C:194:ASP:C	2.64	0.40
2:D:194:ASP:OD1	2:D:194:ASP:C	2.64	0.40
1:A:214:LEU:HD13	1:A:225:ALA:HB1	2.03	0.40
1:B:2:LYS:HA	1:B:90:VAL:O	2.22	0.40
1:B:8:GLU:C	1:B:10:LEU:N	2.79	0.40
1:B:122:TRP:CG	1:B:222:ASN:HD22	2.40	0.40
2:C:2:ILE:N	2:C:2:ILE:CD1	2.83	0.40
2:D:151:VAL:O	2:D:152:ALA:C	2.65	0.40
1:A:7:ARG:O	1:A:7:ARG:CG	2.68	0.40
1:A:130:LEU:HD23	1:A:134:THR:CG2	2.51	0.40
2:C:31:LEU:CD2	2:C:139:CYS:HB2	2.51	0.40
2:C:213:THR:O	2:C:216:HIS:HB2	2.22	0.40
2:C:245:ILE:HD13	2:C:245:ILE:O	2.20	0.40
2:D:299:ARG:HE	2:D:303:GLN:HE21	1.69	0.40
1:A:231:ILE:HD12	1:A:231:ILE:N	2.36	0.40
1:B:42:LEU:HB2	1:B:59:LEU:HD11	2.04	0.40
2:C:153:ALA:O	2:C:156:LYS:N	2.55	0.40
2:C:155:ALA:O	2:C:158:LEU:HB2	2.20	0.40
2:C:250:LEU:O	2:C:254:LEU:HB2	2.21	0.40
2:C:257:LEU:O	2:C:261:LYS:HB2	2.21	0.40
2:D:27:ASP:O	2:D:31:LEU:HG	2.21	0.40
2:D:36:ASP:O	2:D:37:ALA:C	2.64	0.40
2:D:174:TYR:O	2:D:175:GLU:C	2.64	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:315:ASP:OD2	2:D:315:ASP:OD2[2_647]	1.79	0.41
1:A:279:ARG:NH1	2:C:132:ASN:OD1[2_656]	1.81	0.39

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	364/366 (100%)	281 (77%)	62 (17%)	21 (6%)	1	4
1	B	364/366 (100%)	284 (78%)	59 (16%)	21 (6%)	1	4
2	C	322/343 (94%)	234 (73%)	62 (19%)	26 (8%)	1	1
2	D	317/343 (92%)	229 (72%)	69 (22%)	19 (6%)	1	4
All	All	1367/1418 (96%)	1028 (75%)	252 (18%)	87 (6%)	1	3

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	26	THR
1	A	119	LEU
1	B	6	GLU
1	B	26	THR
1	B	119	LEU
1	B	209	GLY
2	C	119	LYS
2	C	131	ALA
2	C	144	GLN
2	C	207	ASN
2	C	270	ARG
2	C	316	TYR
2	D	119	LYS
2	D	131	ALA
2	D	204	GLN

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Mol	Chain	Res	Type
2	D	296	THR
2	D	316	TYR
1	A	94	GLY
1	A	197	ARG
1	A	211	ASP
1	A	220	SER
1	A	277	LYS
1	B	94	GLY
1	B	126	VAL
1	B	156	ASN
1	B	277	LYS
2	C	277	ARG
2	C	278	VAL
2	C	289	ALA
2	C	323	GLU
2	D	75	ALA
2	D	144	GLN
2	D	298	LEU
1	A	121	ASP
1	A	208	ASP
1	A	213	PRO
1	A	287	GLU
1	A	297	PRO
1	A	332	LYS
1	B	25	PRO
1	B	213	PRO
1	B	287	GLU
1	B	297	PRO
1	B	346	SER
2	C	12	GLN
2	C	75	ALA
2	C	227	LYS
2	C	236	LEU
2	C	244	VAL
2	C	283	ARG
2	C	291	ASN
2	D	12	GLN
2	D	61	TRP
2	D	266	HIS
2	D	290	LEU
1	A	25	PRO
1	A	205	ARG

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Mol	Chain	Res	Type
1	B	332	LYS
2	C	105	HIS
2	C	223	MET
2	D	105	HIS
2	D	260	LEU
1	A	84	GLU
1	A	189	PRO
1	A	265	GLN
1	B	84	GLU
1	B	163	GLU
1	B	242	PRO
2	C	61	TRP
2	C	175	GLU
2	C	262	ARG
2	C	312	LEU
2	D	175	GLU
2	D	284	GLY
1	A	117	PRO
1	B	74	LYS
1	B	117	PRO
1	B	265	GLN
2	C	251	GLN
2	C	6	PRO
2	C	56	ASP
2	D	56	ASP
1	A	242	PRO
2	D	6	PRO
1	B	210	GLY
2	D	278	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/311 (100%)	270 (87%)	41 (13%)	4	13
1	B	311/311 (100%)	274 (88%)	37 (12%)	5	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	278/291 (96%)	234 (84%)	44 (16%)	2	8
2	D	276/291 (95%)	240 (87%)	36 (13%)	4	13
All	All	1176/1204 (98%)	1018 (87%)	158 (13%)	4	12

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	6	GLU
1	A	26	THR
1	A	27	LEU
1	A	53	MET
1	A	70	VAL
1	A	73	ARG
1	A	80	ARG
1	A	87	GLU
1	A	96	ARG
1	A	97	MET
1	A	127	GLU
1	A	130	LEU
1	A	131	PRO
1	A	135	MET
1	A	143	GLN
1	A	170	VAL
1	A	172	THR
1	A	176	ARG
1	A	197	ARG
1	A	198	LYS
1	A	202	GLU
1	A	223	ILE
1	A	224	ARG
1	A	226	HIS
1	A	235	LYS
1	A	237	VAL
1	A	253	ASP
1	A	256	LEU
1	A	275	ASN
1	A	278	PHE
1	A	288	ASN
1	A	292	ILE
1	A	293	THR

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Mol	Chain	Res	Type
1	A	297	PRO
1	A	301	GLU
1	A	321	VAL
1	A	339	MET
1	A	342	ASP
1	A	349	ILE
1	A	354	SER
1	B	5	VAL
1	B	6	GLU
1	B	26	THR
1	B	27	LEU
1	B	53	MET
1	B	70	VAL
1	B	73	ARG
1	B	80	ARG
1	B	87	GLU
1	B	96	ARG
1	B	97	MET
1	B	121	ASP
1	B	130	LEU
1	B	135	MET
1	B	146	MET
1	B	162	THR
1	B	169	THR
1	B	176	ARG
1	B	177	LEU
1	B	198	LYS
1	B	202	GLU
1	B	224	ARG
1	B	226	HIS
1	B	235	LYS
1	B	253	ASP
1	B	256	LEU
1	B	275	ASN
1	B	278	PHE
1	B	288	ASN
1	B	292	ILE
1	B	293	THR
1	B	297	PRO
1	B	301	GLU
1	B	321	VAL
1	B	339	MET

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Mol	Chain	Res	Type
1	B	342	ASP
1	B	354	SER
2	C	4	LEU
2	C	17	LEU
2	C	22	LEU
2	C	24	LEU
2	C	79	THR
2	C	82	LEU
2	C	96	GLN
2	C	97	LEU
2	C	110	LEU
2	C	118	SER
2	C	119	LYS
2	C	121	GLN
2	C	132	ASN
2	C	137	VAL
2	C	138	THR
2	C	140	GLN
2	C	143	GLU
2	C	148	PRO
2	C	162	LEU
2	C	173	CYS
2	C	190	LEU
2	C	194	ASP
2	C	203	GLU
2	C	206	VAL
2	C	219	ASP
2	C	227	LYS
2	C	228	ARG
2	C	231	HIS
2	C	234	GLN
2	C	245	ILE
2	C	248	ARG
2	C	249	THR
2	C	251	GLN
2	C	270	ARG
2	C	278	VAL
2	C	293	LEU
2	C	303	GLN
2	C	304	LEU
2	C	312	LEU
2	C	316	TYR

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Mol	Chain	Res	Type
2	C	318	GLN
2	C	325	GLU
2	C	330	LEU
2	C	333	HIS
2	D	2	ILE
2	D	4	LEU
2	D	17	LEU
2	D	22	LEU
2	D	24	LEU
2	D	79	THR
2	D	82	LEU
2	D	96	GLN
2	D	97	LEU
2	D	110	LEU
2	D	118	SER
2	D	119	LYS
2	D	121	GLN
2	D	132	ASN
2	D	137	VAL
2	D	138	THR
2	D	140	GLN
2	D	143	GLU
2	D	148	PRO
2	D	162	LEU
2	D	173	CYS
2	D	190	LEU
2	D	194	ASP
2	D	207	ASN
2	D	208	ASP
2	D	213	THR
2	D	235	GLN
2	D	279	TRP
2	D	292	ARG
2	D	296	THR
2	D	304	LEU
2	D	308	THR
2	D	309	GLU
2	D	311	THR
2	D	316	TYR
2	D	327	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	143	GLN
1	A	186	GLN
1	A	222	ASN
1	A	255	HIS
1	A	265	GLN
1	A	288	ASN
1	A	329	ASN
1	B	61	GLN
1	B	175	HIS
1	B	186	GLN
1	B	226	HIS
1	B	255	HIS
1	B	265	GLN
1	B	288	ASN
1	B	329	ASN
2	C	12	GLN
2	C	35	GLN
2	C	78	GLN
2	C	90	ASN
2	C	94	ASN
2	C	96	GLN
2	C	105	HIS
2	C	140	GLN
2	C	207	ASN
2	C	216	HIS
2	C	251	GLN
2	C	259	ASN
2	C	266	HIS
2	C	303	GLN
2	D	35	GLN
2	D	62	ASN
2	D	69	GLN
2	D	78	GLN
2	D	90	ASN
2	D	94	ASN
2	D	96	GLN
2	D	105	HIS
2	D	140	GLN
2	D	146	GLN
2	D	207	ASN
2	D	231	HIS
2	D	251	GLN

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Mol	Chain	Res	Type
2	D	300	GLN
2	D	303	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	269:LEU	C	270:ARG	N	0.93

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	366/366 (100%)	0.58	32 (8%) 16 13	26, 72, 106, 122	0
1	B	366/366 (100%)	0.80	47 (12%) 7 6	30, 81, 135, 149	0
2	C	328/343 (95%)	0.40	23 (7%) 22 18	21, 60, 132, 168	0
2	D	325/343 (94%)	0.70	30 (9%) 14 12	22, 82, 142, 160	0
All	All	1385/1418 (97%)	0.62	132 (9%) 14 11	21, 73, 132, 168	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	131	ALA	5.9
2	D	318	GLN	4.7
1	B	94	GLY	4.7
1	A	303	GLU	4.7
2	C	225	LYS	4.6
1	A	297	PRO	4.6
1	A	295	ASN	4.1
2	D	164	ASP	4.1
2	D	315	ASP	4.1
2	C	212	PHE	4.1
1	B	53	MET	4.0
2	D	314	GLN	4.0
2	C	315	ASP	4.0
1	B	38	ALA	3.9
1	A	280	GLY	3.9
1	B	10	LEU	3.9
2	D	307	ARG	3.8
1	B	59	LEU	3.7
1	B	49	LEU	3.7
2	C	314	GLN	3.7
1	B	122	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	49	LEU	3.4
1	A	226	HIS	3.4
2	C	318	GLN	3.4
1	A	301	GLU	3.4
1	B	301	GLU	3.4
2	D	268	PRO	3.4
1	B	93	GLU	3.3
1	B	303	GLU	3.2
2	C	294	SER	3.2
1	B	30	LEU	3.2
2	C	210	ALA	3.2
1	B	210	GLY	3.2
1	A	122	TRP	3.1
2	C	269	LEU	3.1
2	C	268	PRO	3.1
1	B	57	VAL	3.0
1	B	32	ASN	3.0
2	D	161	GLU	3.0
2	D	267	THR	3.0
1	A	302	ALA	3.0
1	B	83	PRO	3.0
1	B	27	LEU	3.0
1	A	59	LEU	2.9
1	A	213	PRO	2.9
1	A	314	GLU	2.9
1	B	304	GLU	2.9
2	C	89	PRO	2.9
2	C	316	TYR	2.9
2	D	316	TYR	2.9
1	A	211	ASP	2.9
1	B	71	PRO	2.8
1	B	82	LEU	2.8
2	D	317	GLY	2.8
1	B	36	GLN	2.8
1	B	29	ILE	2.8
1	B	26	THR	2.8
1	B	274	SER	2.8
1	A	28	PRO	2.8
2	D	144	GLN	2.7
1	B	302	ALA	2.7
2	D	13	LEU	2.7
2	D	263	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	286	MET	2.7
1	A	298	GLU	2.7
2	D	175	GLU	2.7
1	B	92	LEU	2.7
1	A	210	GLY	2.7
1	B	67	ALA	2.7
1	A	341	THR	2.7
1	B	37	VAL	2.7
2	D	333	HIS	2.6
1	A	279	ARG	2.6
2	C	279	TRP	2.6
1	B	28	PRO	2.6
1	B	21	LEU	2.6
1	B	60	VAL	2.6
1	A	274	SER	2.5
2	D	285	MET	2.5
2	D	278	VAL	2.5
1	B	86	ALA	2.5
1	B	213	PRO	2.5
2	D	12	GLN	2.5
1	B	108	LEU	2.4
2	D	269	LEU	2.4
1	A	104	SER	2.4
1	B	5	VAL	2.4
2	C	164	ASP	2.4
1	B	9	HIS	2.4
1	B	35	LEU	2.4
1	B	42	LEU	2.4
1	B	209	GLY	2.4
2	C	273	PHE	2.4
2	D	312	LEU	2.4
1	A	62	PRO	2.4
1	A	294	ALA	2.3
2	D	91	ALA	2.3
1	A	92	LEU	2.3
1	B	102	GLY	2.3
1	A	300	GLU	2.3
2	C	48	GLU	2.3
2	C	271	ALA	2.3
2	C	266	HIS	2.3
1	A	284	TYR	2.3
1	A	67	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	121	GLN	2.2
1	B	123	GLN	2.2
2	D	208	ASP	2.2
2	D	262	ARG	2.2
1	B	112	PRO	2.2
2	D	122	GLU	2.2
2	D	272	LEU	2.2
1	A	278	PHE	2.2
1	B	33	LEU	2.2
2	C	161	GLU	2.2
1	A	60	VAL	2.2
2	D	221	LEU	2.1
2	C	296	THR	2.1
1	A	29	ILE	2.1
1	B	101	SER	2.1
1	B	17	VAL	2.1
1	B	20	PRO	2.1
1	B	31	GLY	2.1
2	C	272	LEU	2.1
1	B	231	ILE	2.1
2	D	258	VAL	2.0
2	C	282	ARG	2.0
2	C	267	THR	2.0
1	A	5	VAL	2.0
2	D	260	LEU	2.0
1	A	26	THR	2.0
1	A	225	ALA	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.