



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:46 AM UTC

PDB ID : 1E0K / pdb_00001e0k
Title : gp4d helicase from phage T7
Authors : Singleton, M.R.; Sawaya, M.R.; Ellenberger, T.; Wigley, D.B.
Deposited on : 2000-03-30
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

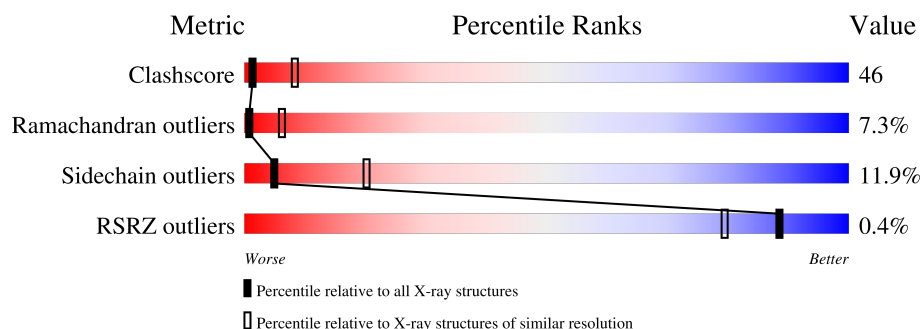
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	289	30%54%13%
1	B	289	34%51%15%
1	C	289	33%54%13%
1	D	289	30%52%16%
1	E	289	33%51%15%
1	F	289	32%54%13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13284 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.

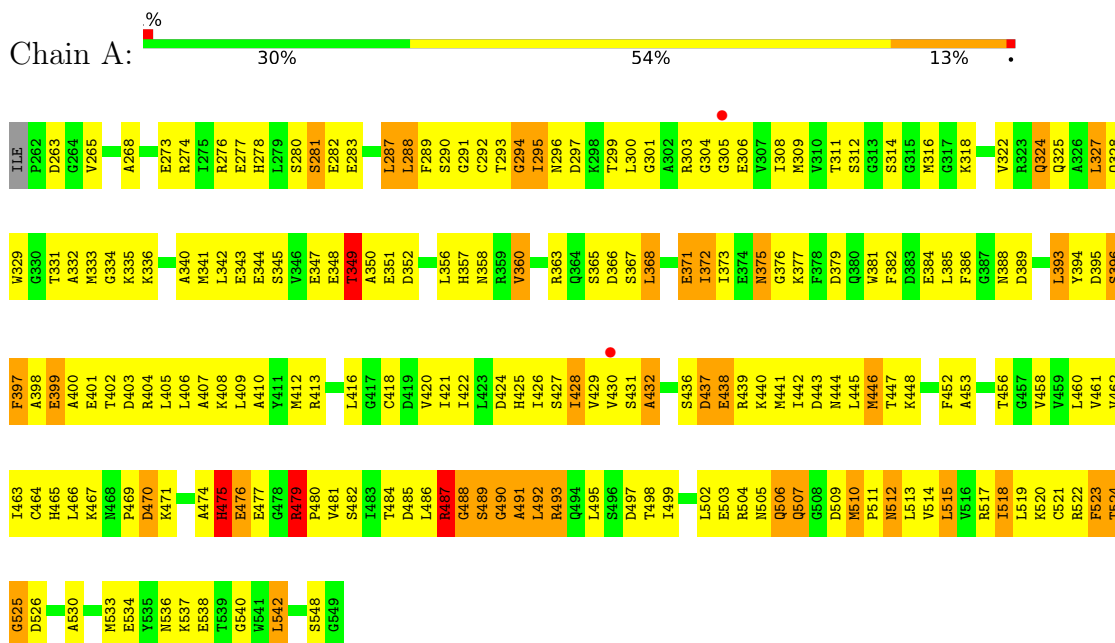
- Molecule 1 is a protein called DNA HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2214	1378	390	433	13			
1	B	288	Total	C	N	O	S	0	0	0
			2214	1378	390	433	13			
1	C	288	Total	C	N	O	S	0	0	0
			2214	1378	390	433	13			
1	D	288	Total	C	N	O	S	0	0	0
			2214	1378	390	433	13			
1	E	288	Total	C	N	O	S	0	0	0
			2214	1378	390	433	13			
1	F	288	Total	C	N	O	S	0	0	0
			2214	1378	390	433	13			

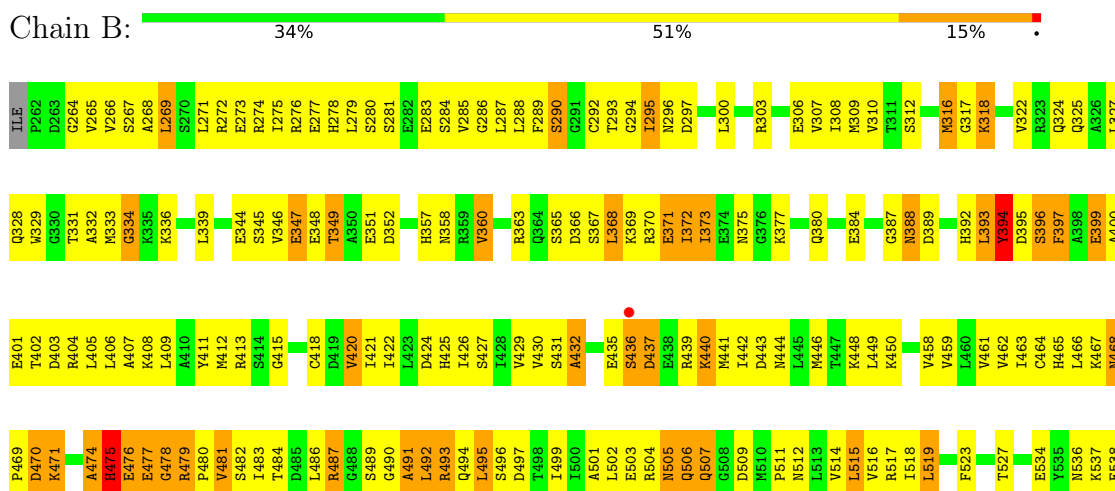
3 Residue-property plots

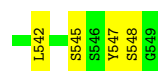
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

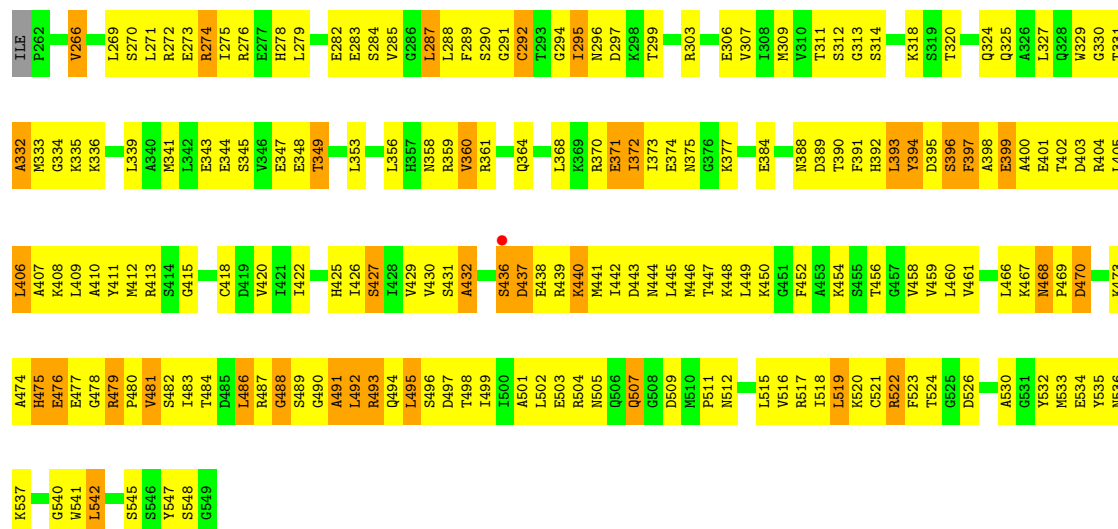


• Molecule 1: DNA HELICASE

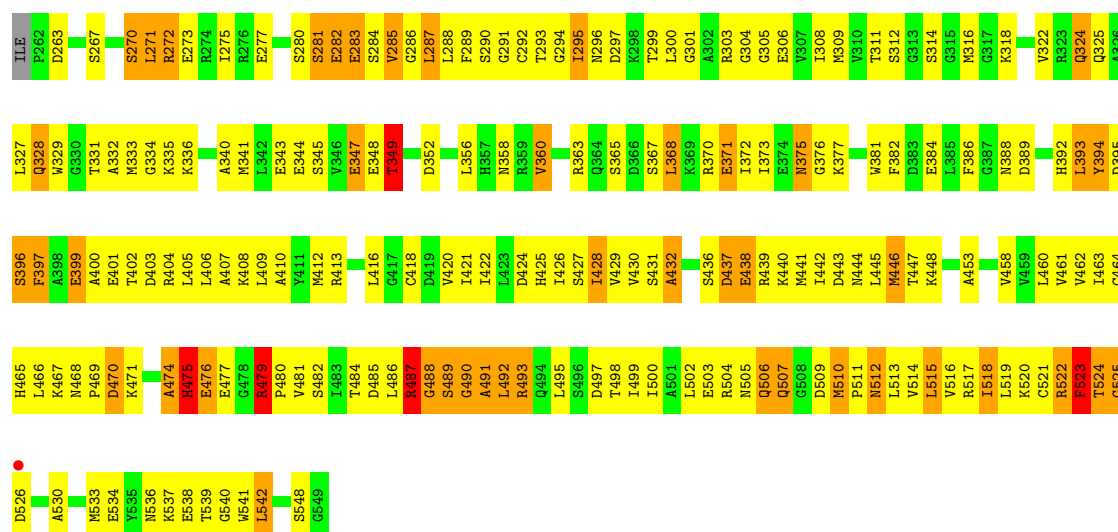




• Molecule 1: DNA HELICASE

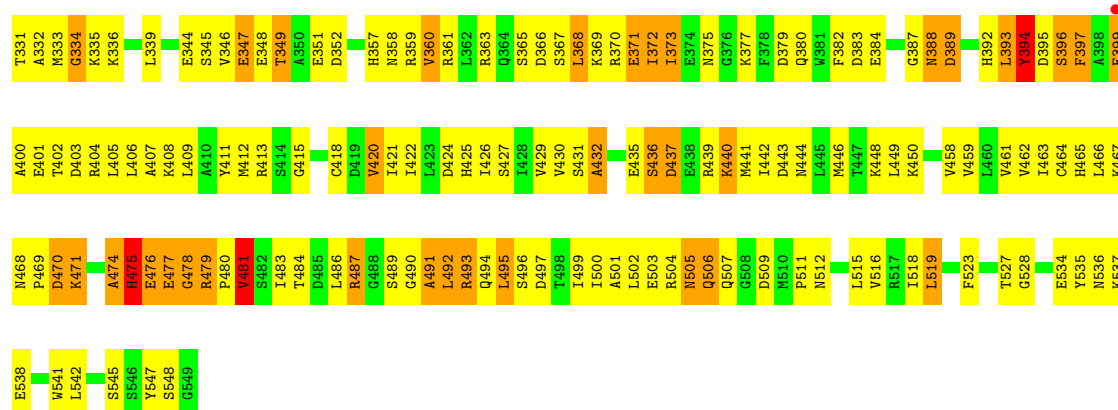


• Molecule 1: DNA HELICASE

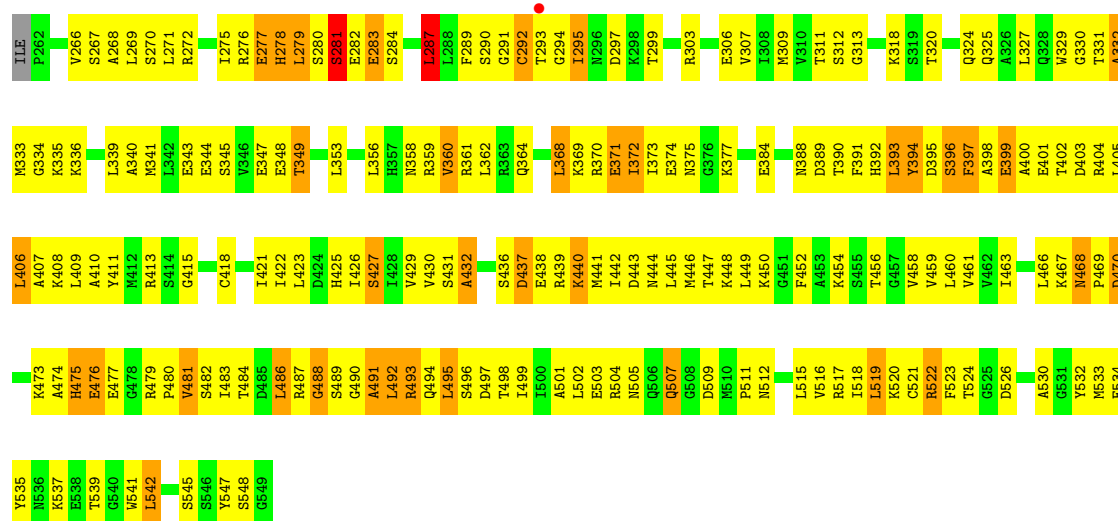


• Molecule 1: DNA HELICASE





- Molecule 1: DNA HELICASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.65Å 120.65Å 284.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-3.30) 94.1 (20.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 3.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.254 , 0.308 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	96.0	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 91.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13284	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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	0.56	0/2243	1.13	21/3011 (0.7%)
1	B	0.59	0/2244	1.14	11/3014 (0.4%)
1	C	0.61	1/2244 (0.0%)	1.15	14/3014 (0.5%)
1	D	0.87	8/2243 (0.4%)	1.19	23/3011 (0.8%)
1	E	0.53	0/2244	1.12	11/3014 (0.4%)
1	F	0.53	0/2244	1.14	13/3014 (0.4%)
All	All	0.63	9/13462 (0.1%)	1.14	93/18078 (0.5%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	283	GLU	N-CA	15.12	1.75	1.46
1	D	523	PHE	CD1-CE1	12.97	1.77	1.38
1	D	523	PHE	CE1-CZ	12.08	1.74	1.38
1	D	523	PHE	CE2-CZ	11.66	1.73	1.38
1	D	523	PHE	CD2-CE2	10.71	1.70	1.38
1	D	282	GLU	C-N	10.60	1.48	1.33
1	D	523	PHE	CG-CD1	7.71	1.55	1.38
1	D	523	PHE	CG-CD2	7.27	1.54	1.38
1	C	412	MET	SD-CE	-5.53	1.65	1.79

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	295	ILE	N-CA-C	-14.58	96.00	110.72
1	D	282	GLU	CA-C-N	14.01	146.91	121.70
1	D	282	GLU	C-N-CA	14.01	146.91	121.70
1	C	295	ILE	N-CA-C	-13.87	96.71	110.72
1	B	295	ILE	N-CA-C	-12.72	95.19	111.09
1	A	295	ILE	N-CA-C	-12.24	98.36	110.72
1	D	295	ILE	N-CA-C	-12.21	98.39	110.72
1	E	295	ILE	N-CA-C	-12.11	95.95	111.09
1	F	491	ALA	N-CA-C	-11.11	99.23	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	474	ALA	N-CA-C	11.07	126.67	109.52
1	B	474	ALA	N-CA-C	10.93	126.46	109.52
1	C	491	ALA	N-CA-C	-10.84	99.56	113.12
1	D	474	ALA	N-CA-C	10.13	126.06	109.95
1	F	427	SER	N-CA-C	-10.05	102.09	114.75
1	C	427	SER	N-CA-C	-9.94	102.23	114.75
1	A	474	ALA	N-CA-C	9.77	125.48	109.95
1	C	474	ALA	N-CA-C	8.84	122.84	109.41
1	F	474	ALA	N-CA-C	8.60	122.47	109.41
1	D	491	ALA	N-CA-C	-7.99	102.44	112.90
1	A	491	ALA	N-CA-C	-7.97	102.45	112.90
1	D	263	ASP	N-CA-C	7.96	123.50	107.41
1	E	478	GLY	N-CA-C	-7.48	99.23	112.77
1	E	283	GLU	N-CA-C	7.38	120.69	108.96
1	E	275	ILE	N-CA-C	-7.36	104.61	111.45
1	A	304	GLY	N-CA-C	-7.33	102.68	112.14
1	B	478	GLY	N-CA-C	-7.27	99.61	112.77
1	F	313	GLY	N-CA-C	-7.22	103.30	112.54
1	E	293	THR	N-CA-C	-7.01	100.07	110.23
1	D	479	ARG	CA-C-N	-6.99	113.50	120.21
1	D	479	ARG	C-N-CA	-6.99	113.50	120.21
1	B	293	THR	N-CA-C	-6.96	100.13	110.23
1	A	479	ARG	CA-C-N	-6.94	113.55	120.21
1	A	479	ARG	C-N-CA	-6.94	113.55	120.21
1	C	313	GLY	N-CA-C	-6.80	103.84	112.54
1	D	304	GLY	N-CA-C	-6.69	103.51	112.14
1	D	291	GLY	N-CA-C	-6.69	105.97	113.79
1	D	318	LYS	N-CA-C	-6.66	104.10	111.36
1	C	409	LEU	N-CA-C	-6.63	104.05	111.28
1	A	318	LYS	N-CA-C	-6.63	104.13	111.36
1	A	393	LEU	N-CA-C	6.59	119.45	109.23
1	D	283	GLU	N-CA-C	6.37	128.84	111.00
1	F	409	LEU	N-CA-C	-6.33	104.38	111.28
1	B	283	GLU	N-CA-C	6.22	118.42	108.41
1	F	283	GLU	N-CA-C	6.16	118.75	108.96
1	A	291	GLY	N-CA-C	-6.11	106.65	113.79
1	D	393	LEU	N-CA-C	6.03	118.58	109.23
1	D	376	GLY	N-CA-C	5.90	123.79	115.30
1	A	372	ILE	N-CA-C	5.88	119.28	111.17
1	D	540	GLY	N-CA-C	-5.82	107.21	115.30
1	F	394	TYR	N-CA-C	-5.77	99.83	109.24
1	C	394	TYR	N-CA-C	-5.76	99.86	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	473	LYS	N-CA-C	-5.75	100.33	109.76
1	C	285	VAL	N-CA-C	-5.67	99.33	107.78
1	B	281	SER	N-CA-C	-5.66	104.10	111.74
1	A	475	HIS	N-CA-C	5.66	122.85	110.80
1	C	473	LYS	N-CA-C	-5.65	100.49	109.76
1	B	491	ALA	N-CA-C	-5.63	103.93	112.04
1	A	263	ASP	N-CA-C	5.60	118.09	109.07
1	E	475	HIS	N-CA-C	5.58	122.69	110.80
1	A	493	ARG	N-CA-C	-5.58	106.45	113.20
1	F	293	THR	N-CA-C	-5.55	102.80	110.35
1	A	376	GLY	N-CA-C	5.54	123.28	115.30
1	D	293	THR	N-CA-C	-5.54	102.28	110.48
1	A	510	MET	CA-C-N	5.51	125.22	119.82
1	A	510	MET	C-N-CA	5.51	125.22	119.82
1	B	475	HIS	N-CA-C	5.48	122.47	110.80
1	B	394	TYR	N-CA-C	-5.44	102.83	110.50
1	E	491	ALA	N-CA-C	-5.42	104.23	112.04
1	A	293	THR	N-CA-C	-5.42	102.46	110.48
1	B	269	LEU	N-CA-C	5.41	117.62	111.02
1	C	540	GLY	N-CA-C	-5.39	107.83	115.43
1	F	468	ASN	CA-C-N	5.37	125.44	119.32
1	F	468	ASN	C-N-CA	5.37	125.44	119.32
1	D	493	ARG	N-CA-C	-5.36	106.72	113.20
1	D	370	ARG	N-CA-C	-5.35	105.34	111.07
1	B	316	MET	N-CA-C	5.32	119.77	113.28
1	C	468	ASN	CA-C-N	5.29	125.36	119.32
1	C	468	ASN	C-N-CA	5.29	125.36	119.32
1	E	481	VAL	N-CA-C	-5.29	102.25	109.55
1	D	349	THR	N-CA-C	-5.26	105.63	111.36
1	C	486	LEU	N-CA-C	5.25	117.93	110.10
1	D	394	TYR	N-CA-C	-5.24	102.72	110.48
1	A	268	ALA	N-CA-C	5.23	119.29	113.01
1	A	349	THR	N-CA-C	-5.23	105.66	111.36
1	D	510	MET	CA-C-N	5.23	124.94	119.82
1	D	510	MET	C-N-CA	5.23	124.94	119.82
1	E	394	TYR	N-CA-C	-5.23	103.13	110.50
1	A	540	GLY	N-CA-C	-5.19	108.08	115.30
1	E	263	ASP	N-CA-C	5.17	117.23	108.02
1	C	269	LEU	N-CA-C	5.09	117.49	111.33
1	F	486	LEU	N-CA-C	5.07	117.65	110.10
1	A	294	GLY	N-CA-C	-5.05	101.21	113.18
1	D	475	HIS	N-CA-C	5.00	121.45	110.80

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	2214	0	2216	190	0
1	B	2214	0	2217	215	0
1	C	2214	0	2217	205	0
1	D	2214	0	2215	242	0
1	E	2214	0	2217	213	0
1	F	2214	0	2217	202	0
All	All	13284	0	13299	1224	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 46.

All (1224) 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:D:523:PHE:CE1	1:D:523:PHE:CD1	1.77	1.66
1:D:523:PHE:CE1	1:D:523:PHE:CZ	1.74	1.65
1:D:283:GLU:N	1:D:523:PHE:CE1	1.70	1.51
1:D:283:GLU:HA	1:D:523:PHE:CE1	1.42	1.50
1:D:283:GLU:N	1:D:283:GLU:CA	1.75	1.50
1:D:283:GLU:CA	1:D:523:PHE:CE1	2.01	1.41
1:D:282:GLU:C	1:D:523:PHE:CE1	2.00	1.37
1:D:282:GLU:C	1:D:523:PHE:CD1	2.11	1.27
1:D:283:GLU:N	1:D:523:PHE:CD1	1.83	1.26
1:D:283:GLU:CA	1:D:523:PHE:CD1	2.20	1.24
1:D:283:GLU:CA	1:D:523:PHE:CZ	2.24	1.18
1:E:290:SER:H	1:E:325:GLN:NE2	1.46	1.12
1:D:477:GLU:HA	1:D:505:ASN:HD22	1.11	1.10
1:A:290:SER:H	1:A:325:GLN:NE2	1.50	1.09
1:A:477:GLU:HA	1:A:505:ASN:HD22	1.14	1.09
1:B:290:SER:H	1:B:325:GLN:NE2	1.50	1.09
1:D:290:SER:H	1:D:325:GLN:NE2	1.52	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:GLU:O	1:D:523:PHE:CE1	2.06	1.06
1:F:290:SER:H	1:F:325:GLN:NE2	1.56	1.04
1:C:290:SER:H	1:C:325:GLN:NE2	1.59	1.01
1:D:283:GLU:C	1:D:523:PHE:CD1	2.40	0.99
1:F:344:GLU:HG3	1:F:349:THR:HG22	1.43	0.99
1:F:406:LEU:HD21	1:F:448:LYS:HB3	1.43	0.99
1:C:406:LEU:HD21	1:C:448:LYS:HB3	1.46	0.97
1:D:425:HIS:HE1	1:D:427:SER:HB2	1.28	0.96
1:D:283:GLU:HA	1:D:523:PHE:CZ	1.97	0.96
1:C:344:GLU:HG3	1:C:349:THR:HG22	1.44	0.96
1:B:440:LYS:HZ2	1:B:444:ASN:HD22	1.12	0.95
1:A:425:HIS:HE1	1:A:427:SER:HB2	1.30	0.94
1:D:282:GLU:O	1:D:523:PHE:CD1	2.18	0.94
1:A:366:ASP:OD1	1:B:284:SER:HB3	1.68	0.93
1:D:283:GLU:HB2	1:D:303:ARG:HD2	1.47	0.93
1:D:412:MET:HE3	1:D:421:ILE:HD12	1.51	0.92
1:F:402:THR:HG23	1:F:445:LEU:HD13	1.51	0.92
1:F:375:ASN:HD21	1:F:377:LYS:HB2	1.34	0.91
1:E:425:HIS:HE1	1:E:427:SER:HB2	1.34	0.91
1:A:412:MET:HE3	1:A:421:ILE:HD12	1.52	0.90
1:E:440:LYS:HZ2	1:E:444:ASN:HD22	1.16	0.90
1:F:518:ILE:HD13	1:F:530:ALA:HB2	1.53	0.90
1:D:290:SER:H	1:D:325:GLN:HE22	1.14	0.90
1:A:290:SER:H	1:A:325:GLN:HE22	1.07	0.90
1:D:477:GLU:HA	1:D:505:ASN:ND2	1.86	0.89
1:D:283:GLU:CA	1:D:523:PHE:CG	2.54	0.89
1:B:476:GLU:O	1:B:506:GLN:HG2	1.72	0.89
1:C:375:ASN:HD21	1:C:377:LYS:HB2	1.37	0.89
1:C:518:ILE:HD13	1:C:530:ALA:HB2	1.55	0.89
1:E:476:GLU:HG3	1:F:483:ILE:HD12	1.54	0.89
1:F:266:VAL:HG11	1:F:271:LEU:HD21	1.52	0.88
1:A:477:GLU:HA	1:A:505:ASN:ND2	1.88	0.88
1:C:402:THR:HG23	1:C:445:LEU:HD13	1.53	0.88
1:D:283:GLU:CA	1:D:523:PHE:CE2	2.55	0.88
1:E:476:GLU:O	1:E:506:GLN:HG2	1.72	0.88
1:E:367:SER:HA	1:E:370:ARG:HH12	1.38	0.88
1:C:290:SER:H	1:C:325:GLN:HE21	1.17	0.87
1:B:476:GLU:HG3	1:C:483:ILE:HD12	1.54	0.87
1:B:425:HIS:HE1	1:B:427:SER:HB2	1.38	0.86
1:D:329:TRP:CZ3	1:D:420:VAL:HG11	2.09	0.86
1:E:478:GLY:O	1:E:479:ARG:HB3	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:HIS:CE1	1:D:427:SER:HB2	2.10	0.86
1:E:393:LEU:N	1:E:393:LEU:HD12	1.91	0.86
1:E:477:GLU:OE2	1:F:482:SER:HB2	1.75	0.86
1:E:425:HIS:CE1	1:E:427:SER:HB2	2.10	0.85
1:A:425:HIS:CE1	1:A:427:SER:HB2	2.11	0.85
1:B:367:SER:HA	1:B:370:ARG:HH12	1.39	0.85
1:B:478:GLY:O	1:B:479:ARG:HB3	1.75	0.85
1:B:393:LEU:N	1:B:393:LEU:HD12	1.91	0.85
1:F:429:VAL:HG23	1:F:430:VAL:H	1.41	0.85
1:C:429:VAL:HG23	1:C:430:VAL:H	1.40	0.84
1:B:440:LYS:NZ	1:B:444:ASN:HD22	1.75	0.84
1:A:329:TRP:CZ3	1:A:420:VAL:HG11	2.12	0.83
1:B:344:GLU:HG3	1:B:349:THR:HG22	1.59	0.83
1:B:474:ALA:HA	1:B:479:ARG:HD2	1.59	0.83
1:B:290:SER:H	1:B:325:GLN:HE21	1.24	0.83
1:A:429:VAL:HG23	1:A:430:VAL:H	1.44	0.82
1:D:518:ILE:CD1	1:D:530:ALA:HB2	2.08	0.82
1:B:440:LYS:O	1:B:440:LYS:HD3	1.80	0.82
1:D:518:ILE:HD11	1:D:530:ALA:HB2	1.58	0.82
1:B:290:SER:N	1:B:325:GLN:NE2	2.28	0.82
1:D:283:GLU:HG2	1:D:284:SER:O	1.78	0.82
1:E:440:LYS:O	1:E:440:LYS:HD3	1.80	0.82
1:F:290:SER:H	1:F:325:GLN:HE21	1.25	0.82
1:B:425:HIS:CE1	1:B:427:SER:HB2	2.14	0.82
1:E:344:GLU:HG3	1:E:349:THR:HG22	1.60	0.82
1:E:440:LYS:NZ	1:E:444:ASN:HD22	1.78	0.82
1:E:474:ALA:HA	1:E:479:ARG:HD2	1.62	0.80
1:D:358:ASN:O	1:D:360:VAL:HG22	1.82	0.80
1:F:327:LEU:HD13	1:F:353:LEU:HD22	1.63	0.80
1:A:477:GLU:OE2	1:B:482:SER:HB2	1.82	0.80
1:C:425:HIS:CE1	1:C:427:SER:HB2	2.16	0.80
1:A:507:GLN:HE21	1:B:517:ARG:HH11	1.27	0.80
1:D:429:VAL:HG23	1:D:430:VAL:H	1.47	0.80
1:A:358:ASN:O	1:A:360:VAL:HG22	1.81	0.79
1:D:283:GLU:CA	1:D:523:PHE:CD2	2.66	0.79
1:E:290:SER:H	1:E:325:GLN:HE22	1.29	0.79
1:E:316:MET:HE1	1:E:503:GLU:HA	1.63	0.79
1:C:266:VAL:HG11	1:C:271:LEU:HD21	1.65	0.79
1:A:518:ILE:CD1	1:A:530:ALA:HB2	2.12	0.78
1:B:477:GLU:HA	1:B:505:ASN:HD22	1.47	0.78
1:E:290:SER:H	1:E:325:GLN:HE21	1.26	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:509:ASP:O	1:F:511:PRO:HD3	1.83	0.78
1:E:285:VAL:HG22	1:E:300:LEU:HD22	1.65	0.78
1:F:358:ASN:O	1:F:360:VAL:HG22	1.83	0.78
1:D:283:GLU:HB2	1:D:303:ARG:CD	2.13	0.78
1:A:375:ASN:HD21	1:A:377:LYS:HG3	1.49	0.78
1:A:518:ILE:HD11	1:A:530:ALA:HB2	1.64	0.78
1:A:288:LEU:N	1:A:288:LEU:HD12	1.99	0.78
1:D:282:GLU:C	1:D:523:PHE:CG	2.37	0.78
1:C:509:ASP:O	1:C:511:PRO:HD3	1.84	0.78
1:F:425:HIS:CE1	1:F:427:SER:HB2	2.18	0.78
1:C:358:ASN:O	1:C:360:VAL:HG22	1.84	0.78
1:A:316:MET:HE3	1:A:504:ARG:H	1.48	0.78
1:B:316:MET:HE1	1:B:503:GLU:HA	1.65	0.77
1:A:517:ARG:HD2	1:A:519:LEU:HD11	1.66	0.77
1:B:289:PHE:H	1:B:296:ASN:HD21	1.33	0.77
1:C:278:HIS:O	1:C:282:GLU:HB2	1.85	0.77
1:C:327:LEU:HD13	1:C:353:LEU:HD22	1.66	0.77
1:C:404:ARG:NH1	1:C:408:LYS:HE3	1.99	0.77
1:D:514:VAL:HG13	1:D:533:MET:HB2	1.67	0.77
1:F:280:SER:O	1:F:281:SER:HB2	1.84	0.77
1:F:404:ARG:NH1	1:F:408:LYS:HE3	2.00	0.77
1:A:426:ILE:O	1:A:426:ILE:HG23	1.84	0.76
1:B:429:VAL:HG23	1:B:430:VAL:H	1.50	0.76
1:D:271:LEU:O	1:D:275:ILE:HG13	1.85	0.76
1:D:517:ARG:HD2	1:D:519:LEU:HD11	1.65	0.76
1:D:283:GLU:CB	1:D:303:ARG:HD2	2.15	0.76
1:D:375:ASN:HD21	1:D:377:LYS:HG3	1.49	0.76
1:D:426:ILE:HG23	1:D:426:ILE:O	1.84	0.76
1:D:283:GLU:CB	1:D:523:PHE:CE2	2.70	0.75
1:E:429:VAL:HG23	1:E:430:VAL:H	1.50	0.75
1:E:477:GLU:HA	1:E:505:ASN:HD22	1.49	0.75
1:D:283:GLU:HG3	1:D:523:PHE:CZ	2.21	0.75
1:D:465:HIS:O	1:D:487:ARG:HB2	1.85	0.75
1:F:287:LEU:HD11	1:F:335:LYS:HG3	1.67	0.75
1:C:287:LEU:HD11	1:C:335:LYS:HG3	1.66	0.75
1:A:446:MET:HG3	1:A:492:LEU:HB3	1.69	0.75
1:A:292:CYS:O	1:A:295:ILE:HD13	1.88	0.74
1:A:316:MET:CE	1:A:504:ARG:H	2.00	0.74
1:B:324:GLN:HE22	1:B:542:LEU:H	1.32	0.73
1:D:316:MET:HE3	1:D:504:ARG:H	1.51	0.73
1:D:446:MET:HG3	1:D:492:LEU:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:GLN:HE22	1:E:542:LEU:H	1.34	0.73
1:A:290:SER:N	1:A:325:GLN:NE2	2.34	0.73
1:A:514:VAL:HG13	1:A:533:MET:HB2	1.70	0.73
1:D:289:PHE:H	1:D:296:ASN:HD21	1.34	0.73
1:A:465:HIS:O	1:A:487:ARG:HB2	1.87	0.73
1:D:480:PRO:HA	1:D:503:GLU:CD	2.14	0.72
1:B:470:ASP:OD2	1:C:467:LYS:NZ	2.23	0.72
1:D:272:ARG:HG2	1:D:273:GLU:N	2.02	0.72
1:E:489:SER:O	1:E:491:ALA:N	2.23	0.72
1:C:446:MET:HE2	1:C:446:MET:HA	1.70	0.72
1:D:282:GLU:CD	1:D:523:PHE:HA	2.14	0.72
1:C:404:ARG:HH12	1:C:408:LYS:CE	2.03	0.72
1:E:328:GLN:HG3	1:E:333:MET:HE3	1.71	0.72
1:B:290:SER:H	1:B:325:GLN:HE22	1.37	0.72
1:C:476:GLU:H	1:C:476:GLU:CD	1.98	0.71
1:B:431:SER:HB3	1:B:441:MET:CE	2.21	0.71
1:B:489:SER:O	1:B:491:ALA:N	2.23	0.71
1:C:429:VAL:HG23	1:C:430:VAL:N	2.05	0.71
1:E:431:SER:HB3	1:E:441:MET:CE	2.21	0.71
1:F:404:ARG:HH12	1:F:408:LYS:HE3	1.56	0.71
1:A:476:GLU:HG3	1:B:483:ILE:HD12	1.73	0.70
1:E:426:ILE:HG12	1:E:426:ILE:O	1.91	0.70
1:F:404:ARG:HH12	1:F:408:LYS:CE	2.04	0.70
1:C:475:HIS:HB2	1:C:476:GLU:OE2	1.92	0.70
1:E:290:SER:N	1:E:325:GLN:NE2	2.31	0.70
1:F:429:VAL:HG23	1:F:430:VAL:N	2.07	0.70
1:F:290:SER:N	1:F:325:GLN:NE2	2.38	0.70
1:F:476:GLU:H	1:F:476:GLU:CD	1.98	0.70
1:F:516:VAL:HG21	1:F:533:MET:CE	2.21	0.70
1:C:290:SER:N	1:C:325:GLN:NE2	2.37	0.70
1:A:480:PRO:HA	1:A:503:GLU:CD	2.16	0.69
1:C:404:ARG:HH12	1:C:408:LYS:HE3	1.55	0.69
1:D:409:LEU:HA	1:D:412:MET:HE2	1.73	0.69
1:F:475:HIS:HB2	1:F:476:GLU:OE2	1.92	0.69
1:E:316:MET:HE3	1:E:504:ARG:N	2.06	0.69
1:F:446:MET:HA	1:F:446:MET:HE2	1.72	0.69
1:C:444:ASN:OD1	1:C:448:LYS:HE2	1.93	0.69
1:A:437:ASP:C	1:A:439:ARG:H	2.00	0.69
1:B:316:MET:CE	1:B:503:GLU:HA	2.23	0.69
1:D:524:THR:C	1:D:526:ASP:H	2.00	0.69
1:B:271:LEU:CD2	1:B:274:ARG:HH21	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:VAL:HG21	1:C:533:MET:HE2	1.75	0.68
1:D:316:MET:CE	1:D:504:ARG:H	2.05	0.68
1:D:329:TRP:HZ3	1:D:420:VAL:HG11	1.57	0.68
1:A:409:LEU:HA	1:A:412:MET:HE2	1.74	0.68
1:C:516:VAL:HG21	1:C:533:MET:CE	2.23	0.68
1:D:292:CYS:O	1:D:295:ILE:HD13	1.94	0.68
1:E:275:ILE:O	1:E:278:HIS:HB3	1.93	0.68
1:F:401:GLU:HB3	1:F:404:ARG:HB2	1.74	0.68
1:B:316:MET:HE3	1:B:504:ARG:N	2.08	0.68
1:E:316:MET:CE	1:E:503:GLU:HA	2.23	0.68
1:E:367:SER:HA	1:E:370:ARG:NH1	2.08	0.68
1:C:284:SER:HB2	1:C:523:PHE:CZ	2.29	0.68
1:E:444:ASN:OD1	1:E:448:LYS:HE2	1.93	0.68
1:F:444:ASN:OD1	1:F:448:LYS:HE2	1.94	0.68
1:B:271:LEU:HD21	1:B:274:ARG:HH21	1.59	0.68
1:A:524:THR:C	1:A:526:ASP:H	2.02	0.68
1:C:399:GLU:HB3	1:C:430:VAL:HG11	1.75	0.68
1:E:345:SER:O	1:E:349:THR:HG23	1.92	0.68
1:C:438:GLU:HA	1:C:441:MET:HG2	1.76	0.68
1:B:367:SER:HA	1:B:370:ARG:NH1	2.09	0.67
1:C:401:GLU:HB3	1:C:404:ARG:HB2	1.75	0.67
1:D:437:ASP:C	1:D:439:ARG:H	2.00	0.67
1:F:336:LYS:HB3	1:F:418:CYS:HA	1.76	0.67
1:F:375:ASN:HD21	1:F:377:LYS:CB	2.04	0.67
1:F:438:GLU:HA	1:F:441:MET:HG2	1.77	0.67
1:D:401:GLU:HA	1:D:430:VAL:O	1.95	0.67
1:F:401:GLU:HA	1:F:430:VAL:O	1.94	0.67
1:E:406:LEU:HD21	1:E:448:LYS:HB3	1.75	0.67
1:F:344:GLU:CG	1:F:349:THR:HG22	2.23	0.67
1:F:452:PHE:CE1	1:F:456:THR:HG21	2.30	0.67
1:C:401:GLU:HA	1:C:430:VAL:O	1.94	0.67
1:F:399:GLU:HB3	1:F:430:VAL:HG11	1.77	0.67
1:C:284:SER:HB2	1:C:523:PHE:HZ	1.59	0.67
1:E:284:SER:HB2	1:E:523:PHE:HZ	1.60	0.66
1:D:402:THR:HG23	1:D:445:LEU:HD13	1.78	0.66
1:D:282:GLU:O	1:D:282:GLU:HG3	1.94	0.66
1:E:450:LYS:HD3	1:E:495:LEU:O	1.96	0.66
1:B:534:GLU:HG3	1:B:545:SER:HB2	1.77	0.66
1:C:294:GLY:HA2	1:C:297:ASP:HB2	1.77	0.66
1:B:444:ASN:OD1	1:B:448:LYS:HE2	1.95	0.66
1:E:331:THR:HG22	1:E:332:ALA:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:536:ASN:C	1:E:536:ASN:HD22	2.02	0.66
1:C:375:ASN:HD21	1:C:377:LYS:CB	2.07	0.66
1:E:344:GLU:HB2	1:E:348:GLU:OE1	1.95	0.66
1:F:481:VAL:HG12	1:F:503:GLU:HG2	1.78	0.66
1:B:426:ILE:HG12	1:B:426:ILE:O	1.95	0.65
1:C:288:LEU:HD12	1:C:288:LEU:H	1.62	0.65
1:D:477:GLU:CA	1:D:505:ASN:HD22	1.99	0.65
1:B:328:GLN:HG3	1:B:333:MET:HE3	1.77	0.65
1:B:406:LEU:HD21	1:B:448:LYS:HB3	1.76	0.65
1:D:476:GLU:HG3	1:E:483:ILE:HD12	1.77	0.65
1:E:327:LEU:HD21	1:E:357:HIS:HA	1.79	0.65
1:C:481:VAL:HG12	1:C:503:GLU:HG2	1.78	0.65
1:D:402:THR:HG21	1:D:448:LYS:NZ	2.12	0.65
1:C:290:SER:N	1:C:325:GLN:HE21	1.93	0.65
1:D:300:LEU:HD12	1:D:524:THR:HG21	1.78	0.65
1:F:294:GLY:HA2	1:F:297:ASP:HB2	1.78	0.65
1:B:331:THR:HG22	1:B:332:ALA:N	2.11	0.64
1:D:340:ALA:C	1:D:341:MET:HE2	2.22	0.64
1:D:476:GLU:O	1:D:506:GLN:HG2	1.97	0.64
1:C:336:LYS:HB3	1:C:418:CYS:HA	1.79	0.64
1:B:290:SER:N	1:B:325:GLN:HE22	1.94	0.64
1:A:401:GLU:HA	1:A:430:VAL:O	1.96	0.64
1:A:476:GLU:O	1:A:506:GLN:HG2	1.97	0.64
1:A:515:LEU:HD23	1:A:515:LEU:C	2.23	0.64
1:E:534:GLU:HG3	1:E:545:SER:HB2	1.78	0.64
1:B:481:VAL:HG11	1:B:501:ALA:HB1	1.78	0.64
1:D:372:ILE:HG21	1:D:381:TRP:CZ3	2.33	0.64
1:E:467:LYS:HE3	1:E:486:LEU:O	1.98	0.64
1:A:402:THR:HG23	1:A:445:LEU:HD13	1.80	0.64
1:E:358:ASN:O	1:E:360:VAL:HG22	1.98	0.64
1:F:344:GLU:HG3	1:F:349:THR:CG2	2.24	0.64
1:B:309:MET:HB3	1:B:499:ILE:HA	1.80	0.63
1:B:450:LYS:HD3	1:B:495:LEU:O	1.99	0.63
1:E:481:VAL:HG11	1:E:501:ALA:HB1	1.78	0.63
1:D:394:TYR:CE1	1:D:408:LYS:HD2	2.34	0.63
1:B:411:TYR:O	1:B:415:GLY:N	2.31	0.63
1:B:412:MET:HE3	1:B:421:ILE:HD12	1.79	0.63
1:F:516:VAL:HG21	1:F:533:MET:HE2	1.81	0.63
1:E:394:TYR:CE2	1:E:408:LYS:HD2	2.34	0.63
1:A:329:TRP:HZ3	1:A:420:VAL:HG11	1.60	0.63
1:B:347:GLU:OE1	1:C:274:ARG:HD2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:HIS:O	1:B:487:ARG:HB2	1.99	0.63
1:C:344:GLU:CG	1:C:349:THR:HG22	2.23	0.63
1:C:375:ASN:ND2	1:C:377:LYS:HB2	2.12	0.63
1:E:316:MET:HG2	1:E:504:ARG:HH11	1.64	0.63
1:A:280:SER:O	1:A:281:SER:HB2	1.99	0.62
1:B:316:MET:HG2	1:B:504:ARG:HG2	1.80	0.62
1:B:316:MET:HG2	1:B:504:ARG:HH11	1.63	0.62
1:D:515:LEU:HD23	1:D:515:LEU:C	2.23	0.62
1:A:394:TYR:CE1	1:A:408:LYS:HD2	2.34	0.62
1:E:470:ASP:OD2	1:F:467:LYS:NZ	2.33	0.62
1:A:309:MET:HB3	1:A:499:ILE:HG12	1.82	0.62
1:C:425:HIS:HE1	1:C:427:SER:HB2	1.63	0.62
1:F:426:ILE:HD12	1:F:446:MET:HE3	1.81	0.62
1:B:345:SER:O	1:B:349:THR:HG23	1.99	0.62
1:C:452:PHE:CE1	1:C:456:THR:HG21	2.34	0.62
1:E:309:MET:HB3	1:E:499:ILE:HA	1.81	0.62
1:F:425:HIS:HE1	1:F:427:SER:HB2	1.64	0.62
1:A:477:GLU:CA	1:A:505:ASN:HD22	2.01	0.62
1:A:518:ILE:N	1:A:518:ILE:HD12	2.15	0.62
1:B:468:ASN:HD21	1:C:493:ARG:CZ	2.11	0.62
1:F:290:SER:N	1:F:325:GLN:HE21	1.96	0.62
1:D:290:SER:N	1:D:325:GLN:HE22	1.93	0.62
1:F:343:GLU:C	1:F:397:PHE:HE1	2.07	0.62
1:A:340:ALA:C	1:A:341:MET:HE2	2.25	0.62
1:C:509:ASP:C	1:C:511:PRO:HD3	2.25	0.62
1:B:273:GLU:OE2	1:B:276:ARG:NH1	2.32	0.62
1:B:394:TYR:CE2	1:B:408:LYS:HD2	2.35	0.62
1:D:280:SER:O	1:D:281:SER:HB2	2.00	0.62
1:E:309:MET:HE2	1:E:464:CYS:HB3	1.82	0.62
1:E:466:LEU:HD21	1:E:486:LEU:HD23	1.81	0.62
1:D:347:GLU:OE1	1:E:274:ARG:HB3	1.99	0.62
1:D:476:GLU:OE1	1:D:476:GLU:N	2.34	0.61
1:D:327:LEU:HD22	1:D:356:LEU:HG	1.82	0.61
1:E:294:GLY:HA2	1:E:297:ASP:HB2	1.82	0.61
1:F:476:GLU:CD	1:F:476:GLU:N	2.57	0.61
1:C:476:GLU:CD	1:C:476:GLU:N	2.57	0.61
1:F:467:LYS:HE3	1:F:486:LEU:O	2.00	0.61
1:B:344:GLU:HB2	1:B:348:GLU:OE1	1.99	0.61
1:E:465:HIS:O	1:E:487:ARG:HB2	2.00	0.61
1:F:375:ASN:ND2	1:F:377:LYS:HB2	2.10	0.61
1:F:402:THR:HG23	1:F:445:LEU:CD1	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:SER:N	1:A:325:GLN:HE22	1.88	0.61
1:B:358:ASN:O	1:B:360:VAL:HG22	2.01	0.61
1:D:309:MET:HB3	1:D:499:ILE:HG12	1.82	0.61
1:B:536:ASN:C	1:B:536:ASN:HD22	2.07	0.61
1:C:467:LYS:HE3	1:C:486:LEU:O	1.99	0.61
1:D:311:THR:HG21	1:D:486:LEU:HD21	1.83	0.61
1:E:411:TYR:O	1:E:415:GLY:N	2.32	0.61
1:E:412:MET:HE3	1:E:421:ILE:HD12	1.82	0.61
1:B:327:LEU:HD21	1:B:357:HIS:HA	1.81	0.61
1:C:344:GLU:HG3	1:C:349:THR:CG2	2.24	0.61
1:A:300:LEU:HD12	1:A:524:THR:HG21	1.81	0.60
1:A:311:THR:HG21	1:A:486:LEU:HD21	1.83	0.60
1:A:422:ILE:HD13	1:A:461:VAL:HB	1.82	0.60
1:D:509:ASP:C	1:D:511:PRO:HD3	2.26	0.60
1:E:394:TYR:CD2	1:E:408:LYS:HD2	2.36	0.60
1:F:320:THR:HG22	1:F:324:GLN:NE2	2.16	0.60
1:F:426:ILE:CD1	1:F:446:MET:HE3	2.31	0.60
1:A:372:ILE:HG21	1:A:381:TRP:CZ3	2.35	0.60
1:A:402:THR:HG21	1:A:448:LYS:NZ	2.16	0.60
1:B:509:ASP:C	1:B:511:PRO:HD3	2.25	0.60
1:E:292:CYS:HB3	1:E:295:ILE:CD1	2.30	0.60
1:F:284:SER:O	1:F:303:ARG:HD2	2.00	0.60
1:B:466:LEU:HD21	1:B:486:LEU:HD23	1.81	0.60
1:B:285:VAL:HG12	1:B:286:GLY:N	2.17	0.60
1:F:312:SER:OG	1:F:318:LYS:HG3	2.00	0.60
1:A:372:ILE:HD13	1:A:381:TRP:CZ3	2.36	0.60
1:D:524:THR:O	1:D:526:ASP:N	2.34	0.60
1:A:476:GLU:N	1:A:476:GLU:OE1	2.34	0.60
1:C:278:HIS:O	1:C:282:GLU:CB	2.49	0.60
1:E:316:MET:HG2	1:E:504:ARG:HG2	1.84	0.60
1:A:350:ALA:HB1	1:B:275:ILE:HD11	1.84	0.60
1:B:371:GLU:O	1:B:373:ILE:N	2.34	0.60
1:C:344:GLU:OE2	1:C:349:THR:HB	2.01	0.60
1:C:484:THR:HA	1:C:493:ARG:NH2	2.16	0.60
1:D:329:TRP:CE3	1:D:420:VAL:HG11	2.36	0.60
1:D:367:SER:O	1:D:371:GLU:HG2	2.01	0.60
1:F:295:ILE:HD11	1:F:516:VAL:HG11	1.84	0.60
1:D:466:LEU:HD13	1:D:475:HIS:CE1	2.37	0.60
1:E:371:GLU:O	1:E:373:ILE:N	2.34	0.60
1:B:426:ILE:CD1	1:B:446:MET:HE3	2.32	0.60
1:C:312:SER:OG	1:C:318:LYS:HG3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:THR:HG21	1:B:448:LYS:NZ	2.17	0.59
1:D:394:TYR:HE1	1:D:408:LYS:HD2	1.67	0.59
1:D:518:ILE:HD12	1:D:518:ILE:N	2.16	0.59
1:E:408:LYS:O	1:E:411:TYR:HB3	2.02	0.59
1:A:329:TRP:CE3	1:A:420:VAL:HG11	2.37	0.59
1:D:372:ILE:HD13	1:D:381:TRP:CZ3	2.37	0.59
1:E:316:MET:HE3	1:E:504:ARG:H	1.66	0.59
1:B:344:GLU:CG	1:B:349:THR:HG22	2.32	0.59
1:E:366:ASP:OD1	1:F:284:SER:HB3	2.02	0.59
1:E:446:MET:SD	1:E:492:LEU:HB3	2.42	0.59
1:E:478:GLY:O	1:E:479:ARG:CB	2.49	0.59
1:F:509:ASP:C	1:F:511:PRO:HD3	2.26	0.59
1:A:509:ASP:C	1:A:511:PRO:HD3	2.27	0.59
1:B:288:LEU:HB3	1:B:296:ASN:OD1	2.03	0.59
1:B:294:GLY:HA2	1:B:297:ASP:HB2	1.85	0.59
1:C:343:GLU:C	1:C:397:PHE:HE1	2.10	0.59
1:C:404:ARG:HH12	1:C:408:LYS:NZ	2.01	0.59
1:D:512:ASN:O	1:D:534:GLU:HA	2.02	0.59
1:A:305:GLY:HA2	1:A:453:ALA:O	2.02	0.59
1:D:422:ILE:HD13	1:D:461:VAL:HB	1.84	0.59
1:B:370:ARG:HH11	1:B:370:ARG:HB3	1.67	0.59
1:B:477:GLU:OE2	1:C:482:SER:HB2	2.02	0.59
1:E:405:LEU:O	1:E:409:LEU:HG	2.03	0.59
1:A:395:ASP:O	1:A:396:SER:HB2	2.02	0.59
1:B:467:LYS:HE3	1:B:486:LEU:O	2.02	0.59
1:A:316:MET:HE3	1:A:504:ARG:N	2.18	0.59
1:E:370:ARG:HH11	1:E:370:ARG:HB3	1.67	0.59
1:E:426:ILE:CD1	1:E:446:MET:HE3	2.33	0.59
1:F:336:LYS:CB	1:F:418:CYS:HA	2.32	0.59
1:F:484:THR:HA	1:F:493:ARG:NH2	2.17	0.59
1:A:309:MET:HE1	1:A:462:VAL:CG1	2.33	0.59
1:A:479:ARG:HG2	1:A:479:ARG:O	2.02	0.59
1:E:402:THR:HG21	1:E:448:LYS:NZ	2.17	0.59
1:F:404:ARG:HH12	1:F:408:LYS:NZ	2.00	0.59
1:A:524:THR:O	1:A:526:ASP:N	2.36	0.58
1:B:394:TYR:CD2	1:B:408:LYS:HD2	2.37	0.58
1:A:488:GLY:O	1:A:490:GLY:N	2.36	0.58
1:E:309:MET:HE3	1:E:462:VAL:O	2.03	0.58
1:E:509:ASP:C	1:E:511:PRO:HD3	2.28	0.58
1:A:352:ASP:O	1:A:356:LEU:HB2	2.03	0.58
1:D:316:MET:CE	1:D:503:GLU:HA	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:365:SER:O	1:E:369:LYS:HG3	2.04	0.58
1:A:309:MET:HE1	1:A:462:VAL:HG12	1.84	0.58
1:A:475:HIS:H	1:A:479:ARG:HD2	1.69	0.58
1:B:466:LEU:CD2	1:B:486:LEU:HD23	2.33	0.58
1:C:405:LEU:O	1:C:406:LEU:C	2.46	0.58
1:D:352:ASP:O	1:D:356:LEU:HB2	2.03	0.58
1:D:536:ASN:O	1:D:538:GLU:N	2.36	0.58
1:A:367:SER:O	1:A:371:GLU:HG2	2.04	0.58
1:C:393:LEU:HD12	1:C:393:LEU:N	2.19	0.58
1:B:309:MET:HE2	1:B:464:CYS:HB3	1.85	0.58
1:B:478:GLY:O	1:B:479:ARG:CB	2.49	0.58
1:E:466:LEU:CD2	1:E:486:LEU:HD23	2.33	0.58
1:D:290:SER:N	1:D:325:GLN:NE2	2.37	0.58
1:A:399:GLU:HB3	1:A:430:VAL:HG21	1.86	0.57
1:B:408:LYS:O	1:B:411:TYR:HB3	2.03	0.57
1:B:493:ARG:O	1:B:493:ARG:HG3	2.04	0.57
1:D:399:GLU:HB3	1:D:430:VAL:HG21	1.86	0.57
1:E:266:VAL:HG11	1:E:271:LEU:HD21	1.85	0.57
1:E:344:GLU:CG	1:E:349:THR:HG22	2.32	0.57
1:E:536:ASN:ND2	1:E:538:GLU:H	2.02	0.57
1:B:405:LEU:O	1:B:409:LEU:HG	2.04	0.57
1:C:371:GLU:O	1:C:374:GLU:N	2.36	0.57
1:C:458:VAL:HG22	1:C:459:VAL:N	2.19	0.57
1:D:425:HIS:H	1:D:463:ILE:HB	1.69	0.57
1:A:536:ASN:O	1:A:538:GLU:N	2.37	0.57
1:F:394:TYR:CE1	1:F:408:LYS:HD2	2.39	0.57
1:A:327:LEU:HD22	1:A:356:LEU:HG	1.84	0.57
1:A:466:LEU:HD13	1:A:475:HIS:CE1	2.40	0.57
1:B:392:HIS:C	1:B:393:LEU:HD12	2.29	0.57
1:A:394:TYR:HE1	1:A:408:LYS:HD2	1.68	0.57
1:A:425:HIS:H	1:A:463:ILE:HB	1.70	0.57
1:C:292:CYS:SG	1:C:295:ILE:CD1	2.92	0.57
1:C:426:ILE:HD12	1:C:446:MET:HE3	1.85	0.57
1:D:282:GLU:N	1:D:523:PHE:CE2	2.72	0.57
1:E:273:GLU:OE2	1:E:276:ARG:NH1	2.37	0.57
1:E:317:GLY:O	1:E:318:LYS:C	2.48	0.57
1:E:351:GLU:OE1	1:F:278:HIS:NE2	2.37	0.57
1:B:292:CYS:HB3	1:B:295:ILE:CD1	2.35	0.57
1:F:345:SER:OG	1:F:348:GLU:HB2	2.04	0.57
1:B:278:HIS:O	1:B:280:SER:N	2.38	0.57
1:C:426:ILE:CD1	1:C:446:MET:HE3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:GLY:O	1:D:490:GLY:N	2.37	0.57
1:F:443:ASP:O	1:F:447:THR:HG23	2.05	0.57
1:F:446:MET:SD	1:F:492:LEU:HB3	2.44	0.57
1:D:395:ASP:O	1:D:396:SER:HB2	2.03	0.57
1:B:285:VAL:HG22	1:B:300:LEU:HD22	1.86	0.56
1:D:475:HIS:H	1:D:479:ARG:HD2	1.69	0.56
1:B:446:MET:SD	1:B:492:LEU:HB3	2.45	0.56
1:D:312:SER:HB2	1:D:502:LEU:O	2.05	0.56
1:D:506:GLN:HB2	1:E:527:THR:OG1	2.04	0.56
1:A:283:GLU:HB3	1:A:303:ARG:HG2	1.88	0.56
1:A:489:SER:O	1:A:491:ALA:N	2.37	0.56
1:C:266:VAL:CG1	1:C:271:LEU:HD21	2.35	0.56
1:D:283:GLU:HB2	1:D:523:PHE:CE2	2.40	0.56
1:D:309:MET:HE1	1:D:462:VAL:CG1	2.36	0.56
1:E:289:PHE:H	1:E:296:ASN:HD21	1.52	0.56
1:F:371:GLU:O	1:F:374:GLU:N	2.37	0.56
1:A:429:VAL:HG23	1:A:430:VAL:N	2.16	0.56
1:C:372:ILE:HA	1:C:375:ASN:OD1	2.06	0.56
1:E:372:ILE:HA	1:E:375:ASN:OD1	2.06	0.56
1:E:399:GLU:HB3	1:E:430:VAL:HG11	1.88	0.56
1:D:480:PRO:HB3	1:D:517:ARG:NH2	2.20	0.56
1:D:489:SER:O	1:D:491:ALA:N	2.38	0.56
1:F:320:THR:CG2	1:F:324:GLN:HE21	2.18	0.56
1:F:422:ILE:HD13	1:F:461:VAL:HB	1.87	0.56
1:C:402:THR:HG23	1:C:445:LEU:CD1	2.29	0.56
1:D:288:LEU:HB3	1:D:296:ASN:OD1	2.05	0.56
1:D:305:GLY:HA2	1:D:453:ALA:O	2.06	0.56
1:E:477:GLU:CA	1:E:505:ASN:HD22	2.18	0.56
1:B:309:MET:HE3	1:B:462:VAL:O	2.05	0.56
1:C:480:PRO:HA	1:C:503:GLU:CD	2.31	0.56
1:D:309:MET:HE1	1:D:462:VAL:HG12	1.86	0.56
1:B:395:ASP:O	1:B:396:SER:HB2	2.06	0.56
1:C:345:SER:OG	1:C:348:GLU:HB2	2.06	0.56
1:B:436:SER:O	1:B:437:ASP:O	2.23	0.56
1:E:436:SER:O	1:E:437:ASP:O	2.24	0.56
1:C:288:LEU:HB3	1:C:296:ASN:CG	2.31	0.55
1:D:479:ARG:O	1:D:479:ARG:HG2	2.04	0.55
1:F:290:SER:H	1:F:325:GLN:HE22	1.50	0.55
1:F:344:GLU:OE2	1:F:349:THR:HB	2.06	0.55
1:F:518:ILE:HD13	1:F:530:ALA:CB	2.34	0.55
1:B:316:MET:HE3	1:B:504:ARG:H	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:LEU:C	1:B:494:GLN:H	2.14	0.55
1:C:394:TYR:CE1	1:C:408:LYS:HD2	2.41	0.55
1:F:327:LEU:HD22	1:F:356:LEU:HD23	1.87	0.55
1:B:317:GLY:O	1:B:318:LYS:C	2.48	0.55
1:B:483:ILE:HG21	1:B:493:ARG:HD3	1.88	0.55
1:D:375:ASN:ND2	1:D:377:LYS:HG3	2.19	0.55
1:E:536:ASN:C	1:E:536:ASN:ND2	2.63	0.55
1:A:316:MET:CE	1:A:503:GLU:HA	2.37	0.55
1:B:375:ASN:HD21	1:B:377:LYS:HD2	1.72	0.55
1:B:536:ASN:ND2	1:B:538:GLU:H	2.05	0.55
1:C:426:ILE:O	1:C:426:ILE:HG12	2.06	0.55
1:E:375:ASN:HD21	1:E:377:LYS:HD2	1.72	0.55
1:E:413:ARG:CD	1:E:458:VAL:HB	2.37	0.55
1:E:484:THR:HA	1:E:493:ARG:NH2	2.21	0.55
1:F:426:ILE:HG12	1:F:426:ILE:O	2.07	0.55
1:A:303:ARG:NH2	1:A:523:PHE:CB	2.69	0.55
1:A:480:PRO:HB3	1:A:517:ARG:NH2	2.21	0.55
1:D:283:GLU:CD	1:D:303:ARG:HD2	2.32	0.55
1:D:294:GLY:HA2	1:D:297:ASP:HB2	1.88	0.55
1:E:290:SER:N	1:E:325:GLN:HE22	1.99	0.55
1:F:372:ILE:HA	1:F:375:ASN:OD1	2.07	0.55
1:F:440:LYS:C	1:F:440:LYS:HD3	2.31	0.55
1:F:480:PRO:HA	1:F:503:GLU:CD	2.31	0.55
1:A:316:MET:CE	1:A:504:ARG:N	2.70	0.55
1:C:336:LYS:CB	1:C:418:CYS:HA	2.37	0.55
1:D:442:ILE:HG23	1:D:443:ASP:N	2.22	0.55
1:E:352:ASP:OD2	1:E:363:ARG:NH2	2.39	0.55
1:F:393:LEU:HD12	1:F:393:LEU:N	2.21	0.55
1:A:350:ALA:CB	1:B:275:ILE:HD11	2.37	0.55
1:B:372:ILE:HA	1:B:375:ASN:OD1	2.07	0.55
1:B:477:GLU:CA	1:B:505:ASN:HD22	2.17	0.55
1:E:360:VAL:HG11	1:E:368:LEU:HD11	1.89	0.55
1:E:469:PRO:O	1:E:470:ASP:C	2.50	0.55
1:D:440:LYS:HD3	1:D:440:LYS:O	2.07	0.55
1:E:493:ARG:HG3	1:E:493:ARG:O	2.06	0.55
1:F:320:THR:CG2	1:F:324:GLN:NE2	2.69	0.55
1:F:458:VAL:HG22	1:F:459:VAL:N	2.22	0.55
1:B:365:SER:O	1:B:369:LYS:HG3	2.07	0.55
1:B:413:ARG:CD	1:B:458:VAL:HB	2.37	0.55
1:C:429:VAL:CG2	1:C:430:VAL:H	2.16	0.55
1:D:386:PHE:CD1	1:E:268:ALA:HB1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:VAL:HG23	1:D:430:VAL:N	2.19	0.55
1:E:483:ILE:HG21	1:E:493:ARG:HD3	1.89	0.55
1:B:400:ALA:O	1:B:430:VAL:HB	2.07	0.54
1:C:295:ILE:HD11	1:C:516:VAL:HG11	1.87	0.54
1:D:283:GLU:HG2	1:D:284:SER:C	2.32	0.54
1:E:392:HIS:C	1:E:393:LEU:HD12	2.31	0.54
1:F:429:VAL:CG2	1:F:430:VAL:H	2.17	0.54
1:A:375:ASN:ND2	1:A:377:LYS:HG3	2.19	0.54
1:F:292:CYS:SG	1:F:295:ILE:CD1	2.95	0.54
1:C:370:ARG:O	1:C:374:GLU:HG3	2.07	0.54
1:C:449:LEU:HD22	1:C:460:LEU:HD21	1.90	0.54
1:D:282:GLU:CA	1:D:523:PHE:CD2	2.87	0.54
1:D:303:ARG:NH2	1:D:523:PHE:CB	2.70	0.54
1:E:307:VAL:HB	1:E:496:SER:HA	1.88	0.54
1:E:394:TYR:CD1	1:E:394:TYR:C	2.85	0.54
1:E:395:ASP:O	1:E:396:SER:HB2	2.07	0.54
1:C:440:LYS:HD3	1:C:440:LYS:C	2.31	0.54
1:E:401:GLU:HA	1:E:430:VAL:O	2.08	0.54
1:A:512:ASN:O	1:A:534:GLU:HA	2.08	0.54
1:B:370:ARG:NH1	1:B:370:ARG:CB	2.71	0.54
1:C:282:GLU:O	1:C:282:GLU:HG3	2.07	0.54
1:A:401:GLU:HB3	1:A:404:ARG:HB2	1.90	0.54
1:A:438:GLU:HA	1:A:441:MET:HG2	1.90	0.54
1:A:536:ASN:C	1:A:538:GLU:N	2.65	0.54
1:B:394:TYR:CD1	1:B:394:TYR:C	2.85	0.54
1:B:413:ARG:HD3	1:B:458:VAL:HB	1.90	0.54
1:B:424:ASP:C	1:B:424:ASP:OD1	2.51	0.54
1:D:316:MET:HE3	1:D:504:ARG:N	2.21	0.54
1:E:471:LYS:O	1:E:471:LYS:HD3	2.07	0.54
1:F:431:SER:O	1:F:432:ALA:C	2.51	0.54
1:D:343:GLU:HG3	1:D:428:ILE:HD11	1.90	0.53
1:E:400:ALA:O	1:E:430:VAL:HB	2.08	0.53
1:C:320:THR:HG22	1:C:324:GLN:NE2	2.24	0.53
1:E:393:LEU:N	1:E:393:LEU:CD1	2.63	0.53
1:E:467:LYS:HG3	1:E:487:ARG:HA	1.90	0.53
1:E:346:VAL:HB	1:E:393:LEU:HD22	1.91	0.53
1:B:399:GLU:HB3	1:B:430:VAL:HG21	1.89	0.53
1:C:405:LEU:O	1:C:407:ALA:N	2.41	0.53
1:C:443:ASP:O	1:C:447:THR:HG23	2.07	0.53
1:D:272:ARG:CG	1:D:273:GLU:N	2.72	0.53
1:D:437:ASP:C	1:D:439:ARG:N	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:331:THR:HG22	1:F:332:ALA:N	2.24	0.53
1:F:405:LEU:O	1:F:406:LEU:C	2.51	0.53
1:F:452:PHE:HE1	1:F:456:THR:HG21	1.74	0.53
1:A:437:ASP:C	1:A:439:ARG:N	2.67	0.53
1:B:307:VAL:HB	1:B:496:SER:HA	1.90	0.53
1:B:399:GLU:HB3	1:B:430:VAL:HG11	1.91	0.53
1:D:524:THR:OG1	1:D:526:ASP:HB3	2.09	0.53
1:A:442:ILE:HG23	1:A:443:ASP:N	2.23	0.53
1:C:345:SER:O	1:C:349:THR:HG23	2.09	0.53
1:D:283:GLU:CB	1:D:523:PHE:CZ	2.92	0.53
1:E:370:ARG:NH1	1:E:370:ARG:CB	2.72	0.53
1:E:480:PRO:HA	1:E:503:GLU:CD	2.33	0.53
1:E:492:LEU:C	1:E:494:GLN:H	2.15	0.53
1:A:343:GLU:HG3	1:A:428:ILE:HD11	1.90	0.53
1:B:471:LYS:HD3	1:B:471:LYS:O	2.08	0.53
1:D:507:GLN:NE2	1:E:528:GLY:HA2	2.23	0.53
1:A:440:LYS:O	1:A:440:LYS:HD3	2.08	0.53
1:E:370:ARG:HH11	1:E:370:ARG:CB	2.22	0.53
1:C:422:ILE:HD13	1:C:461:VAL:HB	1.90	0.52
1:D:514:VAL:CG1	1:D:533:MET:HB2	2.38	0.52
1:F:345:SER:O	1:F:349:THR:HG23	2.09	0.52
1:A:312:SER:HB2	1:A:502:LEU:O	2.10	0.52
1:B:370:ARG:HH11	1:B:370:ARG:CB	2.21	0.52
1:B:404:ARG:O	1:B:408:LYS:HG3	2.09	0.52
1:B:480:PRO:HA	1:B:503:GLU:CD	2.34	0.52
1:E:399:GLU:HB3	1:E:430:VAL:HG21	1.90	0.52
1:E:413:ARG:HD3	1:E:458:VAL:HB	1.90	0.52
1:F:401:GLU:O	1:F:404:ARG:HB3	2.09	0.52
1:F:501:ALA:C	1:F:502:LEU:HD12	2.34	0.52
1:B:440:LYS:NZ	1:B:444:ASN:ND2	2.54	0.52
1:D:283:GLU:C	1:D:523:PHE:CG	2.86	0.52
1:D:327:LEU:CD2	1:D:356:LEU:HG	2.38	0.52
1:D:401:GLU:HB3	1:D:404:ARG:HB2	1.91	0.52
1:D:438:GLU:HA	1:D:441:MET:HG2	1.91	0.52
1:E:492:LEU:C	1:E:494:GLN:N	2.68	0.52
1:B:352:ASP:OD2	1:B:363:ARG:NH2	2.40	0.52
1:A:379:ASP:OD1	1:B:276:ARG:NH2	2.43	0.52
1:B:469:PRO:O	1:B:470:ASP:C	2.51	0.52
1:D:283:GLU:O	1:D:303:ARG:NH1	2.43	0.52
1:F:449:LEU:HD22	1:F:460:LEU:HD21	1.91	0.52
1:B:499:ILE:HB	1:B:519:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:THR:C	1:A:526:ASP:N	2.65	0.52
1:B:303:ARG:O	1:B:306:GLU:HB2	2.09	0.52
1:D:282:GLU:HA	1:D:523:PHE:CD2	2.44	0.52
1:D:372:ILE:HG21	1:D:381:TRP:CH2	2.44	0.52
1:D:444:ASN:O	1:D:447:THR:OG1	2.26	0.52
1:F:489:SER:O	1:F:491:ALA:N	2.43	0.52
1:A:288:LEU:N	1:A:288:LEU:CD1	2.70	0.52
1:A:294:GLY:HA2	1:A:297:ASP:HB2	1.92	0.52
1:B:401:GLU:HA	1:B:430:VAL:O	2.09	0.52
1:C:446:MET:SD	1:C:492:LEU:HB3	2.50	0.52
1:D:375:ASN:ND2	1:D:375:ASN:O	2.43	0.52
1:B:484:THR:HA	1:B:493:ARG:NH2	2.25	0.52
1:B:536:ASN:HD21	1:B:538:GLU:HB2	1.75	0.52
1:E:303:ARG:O	1:E:306:GLU:HB2	2.10	0.52
1:B:467:LYS:HG3	1:B:487:ARG:HA	1.91	0.51
1:B:492:LEU:C	1:B:494:GLN:N	2.67	0.51
1:D:316:MET:HE1	1:D:503:GLU:HA	1.92	0.51
1:D:490:GLY:O	1:D:493:ARG:HG2	2.10	0.51
1:E:499:ILE:HB	1:E:519:LEU:HB3	1.92	0.51
1:E:536:ASN:HD21	1:E:538:GLU:HB2	1.75	0.51
1:B:324:GLN:NE2	1:B:542:LEU:H	2.07	0.51
1:B:360:VAL:HG11	1:B:368:LEU:HD11	1.92	0.51
1:B:396:SER:O	1:B:397:PHE:CB	2.59	0.51
1:C:515:LEU:HD12	1:C:532:TYR:CE2	2.45	0.51
1:F:287:LEU:CD1	1:F:335:LYS:HE3	2.40	0.51
1:A:282:GLU:O	1:A:282:GLU:HG3	2.11	0.51
1:C:517:ARG:HD2	1:C:519:LEU:HD11	1.92	0.51
1:E:518:ILE:HG22	1:E:527:THR:HA	1.92	0.51
1:B:351:GLU:OE1	1:C:278:HIS:NE2	2.42	0.51
1:B:536:ASN:C	1:B:536:ASN:ND2	2.67	0.51
1:C:327:LEU:HD22	1:C:356:LEU:HD23	1.90	0.51
1:C:492:LEU:HD12	1:C:492:LEU:H	1.76	0.51
1:E:442:ILE:HG23	1:E:443:ASP:N	2.26	0.51
1:F:492:LEU:C	1:F:494:GLN:N	2.67	0.51
1:C:489:SER:O	1:C:491:ALA:N	2.43	0.51
1:E:294:GLY:C	1:E:296:ASN:N	2.66	0.51
1:E:404:ARG:O	1:E:408:LYS:HG3	2.11	0.51
1:F:395:ASP:O	1:F:396:SER:HB2	2.10	0.51
1:A:504:ARG:NE	1:A:511:PRO:O	2.33	0.51
1:B:271:LEU:HD21	1:B:274:ARG:NH2	2.24	0.51
1:F:339:LEU:HB3	1:F:341:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:MET:O	1:A:335:LYS:HG2	2.10	0.51
1:A:510:MET:HB3	1:A:513:LEU:HB2	1.93	0.51
1:C:331:THR:HG22	1:C:332:ALA:N	2.25	0.51
1:C:521:CYS:O	1:C:522:ARG:C	2.53	0.51
1:A:524:THR:OG1	1:A:526:ASP:HB3	2.10	0.51
1:C:371:GLU:O	1:C:373:ILE:N	2.44	0.51
1:D:536:ASN:C	1:D:538:GLU:N	2.65	0.51
1:E:383:ASP:CG	1:F:272:ARG:HH22	2.19	0.51
1:F:359:ARG:NH1	1:F:541:TRP:CE2	2.79	0.51
1:F:394:TYR:HE1	1:F:408:LYS:HD2	1.75	0.51
1:C:288:LEU:HB3	1:C:296:ASN:OD1	2.10	0.51
1:F:370:ARG:O	1:F:374:GLU:HG3	2.10	0.51
1:F:492:LEU:HD12	1:F:492:LEU:H	1.75	0.51
1:A:309:MET:HE3	1:A:462:VAL:O	2.11	0.50
1:B:370:ARG:NH1	1:B:370:ARG:HB2	2.26	0.50
1:E:284:SER:HB2	1:E:523:PHE:CZ	2.43	0.50
1:F:406:LEU:CD2	1:F:448:LYS:HB3	2.28	0.50
1:F:411:TYR:CE1	1:F:415:GLY:HA3	2.46	0.50
1:A:265:VAL:HG12	1:A:265:VAL:O	2.11	0.50
1:A:399:GLU:HB3	1:A:430:VAL:HG11	1.94	0.50
1:A:521:CYS:O	1:A:525:GLY:N	2.41	0.50
1:C:288:LEU:HA	1:C:296:ASN:HD21	1.75	0.50
1:C:431:SER:O	1:C:432:ALA:C	2.52	0.50
1:F:517:ARG:HD2	1:F:519:LEU:HD11	1.92	0.50
1:B:324:GLN:HE22	1:B:542:LEU:N	2.06	0.50
1:E:375:ASN:HD21	1:E:377:LYS:CG	2.24	0.50
1:B:442:ILE:HG23	1:B:443:ASP:N	2.26	0.50
1:B:346:VAL:HB	1:B:393:LEU:HD22	1.94	0.50
1:B:409:LEU:HA	1:B:412:MET:HE2	1.94	0.50
1:C:394:TYR:HE1	1:C:408:LYS:HD2	1.77	0.50
1:C:401:GLU:O	1:C:404:ARG:HB3	2.11	0.50
1:C:492:LEU:C	1:C:494:GLN:N	2.68	0.50
1:C:518:ILE:HD13	1:C:530:ALA:CB	2.34	0.50
1:B:265:VAL:HG12	1:B:265:VAL:O	2.12	0.50
1:C:395:ASP:O	1:C:396:SER:HB2	2.12	0.50
1:E:440:LYS:HZ2	1:E:444:ASN:ND2	1.98	0.50
1:F:371:GLU:O	1:F:373:ILE:N	2.44	0.50
1:F:359:ARG:NH1	1:F:541:TRP:CZ2	2.80	0.50
1:B:271:LEU:CD2	1:B:274:ARG:NH2	2.74	0.50
1:C:426:ILE:O	1:C:426:ILE:HG23	2.12	0.50
1:F:306:GLU:HA	1:F:497:ASP:OD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:SER:O	1:B:397:PHE:HB3	2.12	0.49
1:D:283:GLU:CG	1:D:523:PHE:CZ	2.93	0.49
1:F:411:TYR:CD1	1:F:415:GLY:HA3	2.47	0.49
1:A:327:LEU:CD2	1:A:356:LEU:HG	2.42	0.49
1:B:316:MET:HE2	1:B:502:LEU:O	2.11	0.49
1:A:316:MET:HE1	1:A:503:GLU:HA	1.95	0.49
1:A:490:GLY:O	1:A:493:ARG:HG2	2.11	0.49
1:D:267:SER:O	1:D:270:SER:OG	2.22	0.49
1:D:300:LEU:HD12	1:D:524:THR:CG2	2.41	0.49
1:A:536:ASN:C	1:A:538:GLU:H	2.20	0.49
1:B:375:ASN:HD21	1:B:377:LYS:CG	2.25	0.49
1:C:405:LEU:O	1:C:408:LYS:N	2.43	0.49
1:A:303:ARG:NH2	1:A:523:PHE:HB3	2.28	0.49
1:B:440:LYS:HD3	1:B:440:LYS:C	2.37	0.49
1:B:483:ILE:CG2	1:B:493:ARG:HD3	2.42	0.49
1:C:320:THR:CG2	1:C:324:GLN:HE21	2.26	0.49
1:C:396:SER:O	1:C:397:PHE:CB	2.61	0.49
1:D:413:ARG:NH1	1:D:418:CYS:O	2.42	0.49
1:D:536:ASN:C	1:D:538:GLU:H	2.19	0.49
1:E:396:SER:O	1:E:397:PHE:CB	2.59	0.49
1:E:440:LYS:HD3	1:E:440:LYS:C	2.36	0.49
1:F:271:LEU:O	1:F:275:ILE:HG13	2.13	0.49
1:F:469:PRO:O	1:F:470:ASP:C	2.56	0.49
1:B:289:PHE:CD2	1:B:295:ILE:HG22	2.48	0.49
1:C:399:GLU:HB3	1:C:430:VAL:CG1	2.43	0.49
1:C:505:ASN:C	1:C:505:ASN:HD22	2.20	0.49
1:D:467:LYS:HG3	1:D:487:ARG:HA	1.94	0.49
1:D:538:GLU:HA	1:D:538:GLU:OE1	2.13	0.49
1:F:266:VAL:HG11	1:F:271:LEU:CD2	2.35	0.49
1:F:440:LYS:HD3	1:F:440:LYS:O	2.13	0.49
1:A:303:ARG:HH21	1:A:523:PHE:HB2	1.78	0.49
1:A:324:GLN:HE22	1:A:542:LEU:N	2.10	0.49
1:A:518:ILE:CD1	1:A:518:ILE:N	2.76	0.49
1:B:307:VAL:N	1:B:497:ASP:OD2	2.39	0.49
1:D:510:MET:N	1:D:511:PRO:HD3	2.28	0.49
1:E:308:ILE:HB	1:E:461:VAL:HA	1.95	0.49
1:E:316:MET:HE2	1:E:502:LEU:O	2.12	0.49
1:E:396:SER:O	1:E:397:PHE:HB3	2.13	0.49
1:A:358:ASN:ND2	1:A:381:TRP:NE1	2.60	0.49
1:A:467:LYS:HG3	1:A:487:ARG:HA	1.94	0.49
1:C:406:LEU:CD2	1:C:448:LYS:HB3	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:392:HIS:C	1:F:393:LEU:HD12	2.38	0.49
1:A:299:THR:O	1:A:300:LEU:HB2	2.12	0.49
1:F:426:ILE:O	1:F:426:ILE:HG23	2.12	0.49
1:B:440:LYS:HZ2	1:B:444:ASN:ND2	1.95	0.48
1:B:475:HIS:CD2	1:B:479:ARG:HD3	2.47	0.48
1:C:449:LEU:O	1:C:452:PHE:HB3	2.13	0.48
1:C:501:ALA:C	1:C:502:LEU:HD12	2.38	0.48
1:E:440:LYS:NZ	1:E:444:ASN:ND2	2.56	0.48
1:E:483:ILE:CG2	1:E:493:ARG:HD3	2.43	0.48
1:A:300:LEU:HD12	1:A:524:THR:CG2	2.43	0.48
1:A:538:GLU:OE1	1:A:538:GLU:HA	2.11	0.48
1:B:294:GLY:C	1:B:296:ASN:N	2.64	0.48
1:B:393:LEU:N	1:B:393:LEU:CD1	2.62	0.48
1:C:287:LEU:HG	1:C:329:TRP:CD1	2.48	0.48
1:D:283:GLU:HB2	1:D:303:ARG:NE	2.27	0.48
1:D:299:THR:O	1:D:300:LEU:HB2	2.12	0.48
1:F:517:ARG:HD2	1:F:519:LEU:CD1	2.43	0.48
1:B:429:VAL:HG23	1:B:430:VAL:N	2.24	0.48
1:C:327:LEU:HD13	1:C:353:LEU:CD2	2.41	0.48
1:D:303:ARG:NH2	1:D:523:PHE:HB3	2.28	0.48
1:E:429:VAL:HG23	1:E:430:VAL:N	2.23	0.48
1:A:283:GLU:O	1:A:306:GLU:OE2	2.30	0.48
1:B:268:ALA:O	1:B:271:LEU:HB2	2.13	0.48
1:B:344:GLU:HG3	1:B:349:THR:CG2	2.39	0.48
1:C:306:GLU:HA	1:C:497:ASP:OD2	2.13	0.48
1:C:517:ARG:HD2	1:C:519:LEU:CD1	2.43	0.48
1:D:480:PRO:HB3	1:D:517:ARG:HH21	1.79	0.48
1:F:292:CYS:SG	1:F:295:ILE:HD13	2.53	0.48
1:A:506:GLN:HB2	1:B:527:THR:OG1	2.14	0.48
1:C:291:GLY:O	1:C:292:CYS:HB2	2.13	0.48
1:C:359:ARG:NH1	1:C:541:TRP:CE2	2.82	0.48
1:A:372:ILE:HG21	1:A:381:TRP:CH2	2.48	0.48
1:B:267:SER:O	1:B:268:ALA:C	2.57	0.48
1:C:440:LYS:HD3	1:C:440:LYS:O	2.14	0.48
1:C:452:PHE:HE1	1:C:456:THR:HG21	1.78	0.48
1:E:370:ARG:NH1	1:E:370:ARG:HB2	2.28	0.48
1:E:426:ILE:O	1:E:426:ILE:CG1	2.61	0.48
1:F:396:SER:O	1:F:397:PHE:CB	2.61	0.48
1:F:405:LEU:O	1:F:407:ALA:N	2.47	0.48
1:C:339:LEU:HB3	1:C:341:MET:HE3	1.95	0.48
1:D:316:MET:CE	1:D:504:ARG:N	2.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:467:LYS:CG	1:E:487:ARG:HA	2.44	0.48
1:A:510:MET:N	1:A:511:PRO:HD3	2.29	0.48
1:B:310:VAL:HG11	1:B:322:VAL:HG23	1.95	0.48
1:B:316:MET:CG	1:B:504:ARG:HH11	2.27	0.48
1:D:480:PRO:HA	1:D:503:GLU:OE2	2.14	0.48
1:F:505:ASN:HD22	1:F:505:ASN:C	2.20	0.48
1:D:324:GLN:HE22	1:D:542:LEU:N	2.11	0.48
1:D:413:ARG:HD3	1:D:458:VAL:HB	1.96	0.48
1:D:477:GLU:CA	1:D:505:ASN:ND2	2.68	0.48
1:D:510:MET:HB3	1:D:513:LEU:HB2	1.95	0.48
1:F:440:LYS:HZ3	1:F:444:ASN:HB2	1.78	0.48
1:C:361:ARG:HB3	1:C:364:GLN:OE1	2.14	0.48
1:D:388:ASN:O	1:D:389:ASP:C	2.56	0.48
1:D:399:GLU:HB3	1:D:430:VAL:HG11	1.95	0.48
1:D:468:ASN:HD21	1:E:493:ARG:HD2	1.79	0.48
1:E:310:VAL:HG11	1:E:322:VAL:HG23	1.94	0.48
1:A:273:GLU:OE1	1:A:276:ARG:NH1	2.47	0.47
1:B:439:ARG:O	1:B:442:ILE:HG22	2.14	0.47
1:C:320:THR:CG2	1:C:324:GLN:NE2	2.77	0.47
1:D:431:SER:O	1:D:432:ALA:C	2.56	0.47
1:D:437:ASP:O	1:D:439:ARG:N	2.47	0.47
1:E:327:LEU:HD21	1:E:357:HIS:CA	2.43	0.47
1:F:521:CYS:O	1:F:522:ARG:C	2.57	0.47
1:A:289:PHE:HA	1:A:325:GLN:HE21	1.79	0.47
1:B:435:GLU:O	1:B:436:SER:O	2.33	0.47
1:C:411:TYR:CE1	1:C:415:GLY:HA3	2.49	0.47
1:D:309:MET:HE3	1:D:462:VAL:O	2.14	0.47
1:E:324:GLN:NE2	1:E:542:LEU:H	2.08	0.47
1:E:439:ARG:O	1:E:442:ILE:HG22	2.14	0.47
1:B:308:ILE:HB	1:B:461:VAL:HA	1.96	0.47
1:D:389:ASP:HB2	1:E:269:LEU:HD12	1.97	0.47
1:D:502:LEU:HD23	1:D:514:VAL:HG21	1.96	0.47
1:E:401:GLU:HB3	1:E:404:ARG:HB2	1.96	0.47
1:F:275:ILE:O	1:F:278:HIS:HB3	2.14	0.47
1:F:446:MET:HE2	1:F:449:LEU:HD12	1.96	0.47
1:A:375:ASN:ND2	1:A:375:ASN:O	2.45	0.47
1:C:469:PRO:O	1:C:470:ASP:C	2.56	0.47
1:D:284:SER:O	1:D:285:VAL:HG23	2.14	0.47
1:D:498:THR:HG23	1:D:520:LYS:O	2.15	0.47
1:E:329:TRP:CZ3	1:E:420:VAL:HG11	2.49	0.47
1:F:307:VAL:HB	1:F:496:SER:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:405:LEU:O	1:F:408:LYS:N	2.45	0.47
1:F:518:ILE:O	1:F:518:ILE:HG22	2.14	0.47
1:A:388:ASN:O	1:A:389:ASP:C	2.57	0.47
1:B:346:VAL:CG2	1:C:271:LEU:HD13	2.44	0.47
1:D:482:SER:OG	1:D:484:THR:OG1	2.32	0.47
1:E:435:GLU:O	1:E:436:SER:O	2.32	0.47
1:F:516:VAL:HG21	1:F:533:MET:HE3	1.96	0.47
1:B:467:LYS:CG	1:B:487:ARG:HA	2.45	0.47
1:C:331:THR:O	1:C:334:GLY:N	2.39	0.47
1:E:328:GLN:CG	1:E:333:MET:HE3	2.43	0.47
1:E:424:ASP:OD1	1:E:424:ASP:C	2.57	0.47
1:F:388:ASN:O	1:F:389:ASP:C	2.58	0.47
1:A:278:HIS:O	1:A:282:GLU:HB2	2.15	0.47
1:A:431:SER:O	1:A:432:ALA:C	2.56	0.47
1:B:370:ARG:O	1:B:373:ILE:HB	2.15	0.47
1:B:401:GLU:HB3	1:B:404:ARG:HB2	1.97	0.47
1:B:426:ILE:HD13	1:B:446:MET:HE3	1.97	0.47
1:C:292:CYS:SG	1:C:295:ILE:HD13	2.55	0.47
1:C:359:ARG:NH1	1:C:541:TRP:CZ2	2.83	0.47
1:C:398:ALA:O	1:C:399:GLU:C	2.58	0.47
1:D:402:THR:HG21	1:D:448:LYS:HZ1	1.79	0.47
1:E:333:MET:O	1:E:335:LYS:HG2	2.15	0.47
1:F:299:THR:O	1:F:303:ARG:NH1	2.40	0.47
1:F:399:GLU:HB3	1:F:430:VAL:HG21	1.96	0.47
1:B:507:GLN:HE21	1:C:517:ARG:HH11	1.63	0.47
1:D:407:ALA:O	1:D:410:ALA:HB3	2.14	0.47
1:D:518:ILE:CD1	1:D:518:ILE:N	2.78	0.47
1:E:492:LEU:HD12	1:E:493:ARG:H	1.79	0.47
1:C:491:ALA:O	1:C:495:LEU:HD22	2.15	0.47
1:E:324:GLN:HE22	1:E:542:LEU:N	2.07	0.47
1:E:475:HIS:CD2	1:E:479:ARG:HD3	2.49	0.47
1:F:289:PHE:CD2	1:F:295:ILE:CG2	2.98	0.47
1:A:396:SER:O	1:A:397:PHE:CB	2.62	0.47
1:E:382:PHE:CE2	1:F:272:ARG:HG3	2.50	0.47
1:F:524:THR:C	1:F:526:ASP:H	2.23	0.47
1:A:437:ASP:O	1:A:439:ARG:N	2.48	0.46
1:B:371:GLU:C	1:B:373:ILE:N	2.73	0.46
1:B:492:LEU:HD12	1:B:493:ARG:H	1.79	0.46
1:C:388:ASN:O	1:C:389:ASP:C	2.57	0.46
1:D:283:GLU:O	1:D:299:THR:O	2.32	0.46
1:E:316:MET:CE	1:E:504:ARG:H	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:VAL:CG1	1:A:533:MET:HB2	2.43	0.46
1:C:405:LEU:C	1:C:407:ALA:N	2.73	0.46
1:D:375:ASN:ND2	1:D:375:ASN:C	2.73	0.46
1:D:396:SER:O	1:D:397:PHE:CB	2.63	0.46
1:E:446:MET:HE2	1:E:449:LEU:HD12	1.96	0.46
1:A:502:LEU:HD23	1:A:514:VAL:HG21	1.97	0.46
1:C:276:ARG:C	1:C:278:HIS:N	2.73	0.46
1:D:375:ASN:HD21	1:D:377:LYS:CG	2.23	0.46
1:C:399:GLU:HB3	1:C:430:VAL:HG21	1.96	0.46
1:D:521:CYS:O	1:D:525:GLY:N	2.41	0.46
1:E:289:PHE:CD2	1:E:295:ILE:HG22	2.50	0.46
1:E:303:ARG:NH2	1:E:523:PHE:HB3	2.31	0.46
1:A:336:LYS:CB	1:A:418:CYS:HA	2.46	0.46
1:E:287:LEU:HD11	1:E:335:LYS:HE2	1.96	0.46
1:E:339:LEU:O	1:E:393:LEU:HA	2.14	0.46
1:F:515:LEU:HD12	1:F:532:TYR:CE2	2.50	0.46
1:A:331:THR:HG22	1:A:332:ALA:N	2.29	0.46
1:A:480:PRO:HB3	1:A:517:ARG:HH21	1.81	0.46
1:F:399:GLU:HB3	1:F:430:VAL:CG1	2.44	0.46
1:F:413:ARG:HD3	1:F:458:VAL:HB	1.98	0.46
1:B:351:GLU:HG3	1:C:279:LEU:HD21	1.98	0.46
1:D:308:ILE:HD13	1:D:308:ILE:N	2.30	0.46
1:D:358:ASN:ND2	1:D:381:TRP:NE1	2.63	0.46
1:D:394:TYR:OH	1:D:400:ALA:HB2	2.16	0.46
1:D:506:GLN:HG2	1:D:506:GLN:H	1.56	0.46
1:D:507:GLN:HE22	1:E:528:GLY:HA2	1.81	0.46
1:A:295:ILE:HD12	1:A:295:ILE:N	2.30	0.46
1:A:444:ASN:O	1:A:447:THR:OG1	2.26	0.46
1:A:477:GLU:CA	1:A:505:ASN:ND2	2.70	0.46
1:B:431:SER:O	1:B:432:ALA:C	2.59	0.46
1:D:515:LEU:C	1:D:515:LEU:CD2	2.89	0.46
1:B:285:VAL:CG1	1:B:286:GLY:N	2.79	0.46
1:D:345:SER:OG	1:D:348:GLU:HG3	2.16	0.46
1:D:392:HIS:ND1	1:E:267:SER:HB2	2.31	0.46
1:D:405:LEU:HD11	1:D:409:LEU:HD21	1.97	0.46
1:D:426:ILE:HG22	1:D:464:CYS:HB3	1.97	0.46
1:E:316:MET:CG	1:E:504:ARG:HH11	2.28	0.46
1:E:370:ARG:O	1:E:373:ILE:HB	2.16	0.46
1:D:282:GLU:N	1:D:523:PHE:CZ	2.84	0.46
1:B:295:ILE:HG13	1:B:516:VAL:HG11	1.98	0.45
1:B:346:VAL:HG21	1:C:271:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:ILE:N	1:D:295:ILE:HD12	2.32	0.45
1:D:399:GLU:OE1	1:D:430:VAL:HG22	2.16	0.45
1:E:344:GLU:HG3	1:E:349:THR:CG2	2.39	0.45
1:F:361:ARG:HB3	1:F:364:GLN:OE1	2.16	0.45
1:A:469:PRO:O	1:A:470:ASP:C	2.59	0.45
1:B:339:LEU:O	1:B:393:LEU:HA	2.16	0.45
1:C:400:ALA:O	1:C:430:VAL:HB	2.16	0.45
1:C:534:GLU:HG3	1:C:545:SER:HB2	1.99	0.45
1:D:368:LEU:HA	1:D:371:GLU:HG3	1.98	0.45
1:E:401:GLU:HG2	1:E:402:THR:H	1.81	0.45
1:F:502:LEU:HD12	1:F:502:LEU:N	2.31	0.45
1:F:503:GLU:OE1	1:F:515:LEU:HD22	2.16	0.45
1:A:336:LYS:HB2	1:A:418:CYS:HA	1.98	0.45
1:A:421:ILE:HB	1:A:460:LEU:HD12	1.98	0.45
1:B:425:HIS:H	1:B:463:ILE:HB	1.82	0.45
1:D:336:LYS:HB2	1:D:418:CYS:HA	1.98	0.45
1:D:504:ARG:NE	1:D:511:PRO:O	2.34	0.45
1:F:535:TYR:HD1	1:F:542:LEU:HD12	1.81	0.45
1:A:351:GLU:OE1	1:B:278:HIS:NE2	2.46	0.45
1:C:503:GLU:OE1	1:C:515:LEU:HD22	2.16	0.45
1:D:303:ARG:HH21	1:D:523:PHE:HB2	1.81	0.45
1:D:466:LEU:HD23	1:D:486:LEU:HA	1.99	0.45
1:F:266:VAL:CG1	1:F:270:SER:OG	2.65	0.45
1:F:400:ALA:O	1:F:430:VAL:HB	2.16	0.45
1:A:344:GLU:HG3	1:A:349:THR:HG22	1.99	0.45
1:B:329:TRP:CZ3	1:B:420:VAL:HG11	2.51	0.45
1:C:467:LYS:O	1:C:469:PRO:HD3	2.16	0.45
1:D:306:GLU:HG2	1:D:497:ASP:HB2	1.98	0.45
1:D:344:GLU:HG3	1:D:349:THR:HG22	1.97	0.45
1:E:402:THR:HG21	1:E:448:LYS:HZ1	1.80	0.45
1:B:468:ASN:OD1	1:C:493:ARG:NH2	2.49	0.45
1:C:535:TYR:HD1	1:C:542:LEU:HD12	1.82	0.45
1:E:348:GLU:O	1:E:351:GLU:HB3	2.16	0.45
1:E:422:ILE:HD13	1:E:461:VAL:HB	1.98	0.45
1:F:450:LYS:HD2	1:F:450:LYS:O	2.16	0.45
1:F:537:LYS:HE2	1:F:537:LYS:HB3	1.76	0.45
1:B:266:VAL:HG12	1:B:267:SER:N	2.32	0.45
1:B:333:MET:O	1:B:334:GLY:C	2.59	0.45
1:B:422:ILE:HD13	1:B:461:VAL:HB	1.98	0.45
1:D:469:PRO:O	1:D:470:ASP:C	2.59	0.45
1:E:333:MET:O	1:E:334:GLY:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:371:GLU:C	1:E:373:ILE:N	2.73	0.45
1:F:466:LEU:HB3	1:F:475:HIS:HE1	1.82	0.45
1:A:375:ASN:HD21	1:A:377:LYS:CG	2.23	0.45
1:C:276:ARG:HB2	1:C:276:ARG:NH1	2.32	0.45
1:C:330:GLY:HA3	1:C:391:PHE:CZ	2.52	0.45
1:C:413:ARG:HD3	1:C:458:VAL:HB	1.99	0.45
1:C:437:ASP:C	1:C:439:ARG:H	2.25	0.45
1:D:336:LYS:CB	1:D:418:CYS:HA	2.45	0.45
1:D:421:ILE:HB	1:D:460:LEU:HD12	1.99	0.45
1:D:424:ASP:OD1	1:D:424:ASP:C	2.60	0.45
1:E:426:ILE:HD13	1:E:446:MET:HE3	1.99	0.45
1:A:308:ILE:N	1:A:308:ILE:HD13	2.32	0.45
1:A:375:ASN:ND2	1:A:375:ASN:C	2.74	0.45
1:B:366:ASP:OD1	1:C:284:SER:OG	2.33	0.45
1:B:466:LEU:HD23	1:B:486:LEU:HA	1.98	0.45
1:C:440:LYS:HZ3	1:C:444:ASN:HB2	1.82	0.45
1:E:431:SER:O	1:E:432:ALA:C	2.59	0.45
1:F:411:TYR:O	1:F:415:GLY:N	2.45	0.45
1:A:306:GLU:HG2	1:A:497:ASP:HB2	1.99	0.44
1:A:426:ILE:O	1:A:426:ILE:CG2	2.56	0.44
1:A:466:LEU:CD2	1:A:486:LEU:HD23	2.47	0.44
1:A:466:LEU:HD23	1:A:486:LEU:HA	1.99	0.44
1:B:518:ILE:HG22	1:B:527:THR:HA	1.99	0.44
1:C:446:MET:HE2	1:C:449:LEU:HD12	1.99	0.44
1:D:426:ILE:O	1:D:426:ILE:CG2	2.57	0.44
1:E:295:ILE:HG13	1:E:516:VAL:HG11	1.99	0.44
1:F:330:GLY:HA3	1:F:391:PHE:CZ	2.53	0.44
1:B:404:ARG:O	1:B:407:ALA:HB3	2.17	0.44
1:D:303:ARG:HB2	1:D:306:GLU:OE2	2.17	0.44
1:F:492:LEU:H	1:F:492:LEU:CD1	2.29	0.44
1:B:275:ILE:O	1:B:275:ILE:CG2	2.64	0.44
1:B:401:GLU:HG2	1:B:402:THR:H	1.83	0.44
1:B:446:MET:HE2	1:B:449:LEU:HD12	1.97	0.44
1:D:519:LEU:O	1:D:520:LYS:HB2	2.17	0.44
1:F:309:MET:HB3	1:F:499:ILE:HA	2.00	0.44
1:F:491:ALA:O	1:F:495:LEU:HD22	2.18	0.44
1:A:413:ARG:NH1	1:A:418:CYS:O	2.41	0.44
1:B:402:THR:HG21	1:B:448:LYS:HZ2	1.80	0.44
1:C:375:ASN:HD21	1:C:377:LYS:CG	2.31	0.44
1:C:392:HIS:C	1:C:393:LEU:HD12	2.41	0.44
1:C:492:LEU:H	1:C:492:LEU:CD1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:LEU:HD23	1:E:486:LEU:HA	1.99	0.44
1:F:375:ASN:HD21	1:F:377:LYS:CG	2.29	0.44
1:F:398:ALA:O	1:F:399:GLU:C	2.60	0.44
1:A:399:GLU:OE1	1:A:430:VAL:HG22	2.16	0.44
1:B:367:SER:O	1:B:371:GLU:HG2	2.18	0.44
1:B:431:SER:HB3	1:B:441:MET:HE1	1.98	0.44
1:E:272:ARG:HG2	1:E:273:GLU:N	2.31	0.44
1:F:289:PHE:CD2	1:F:295:ILE:HG22	2.52	0.44
1:F:439:ARG:O	1:F:442:ILE:HG22	2.17	0.44
1:F:534:GLU:HG3	1:F:545:SER:HB2	1.99	0.44
1:A:288:LEU:HB3	1:A:296:ASN:CG	2.43	0.44
1:C:270:SER:C	1:C:271:LEU:HD23	2.42	0.44
1:D:365:SER:OG	1:D:368:LEU:HB2	2.17	0.44
1:E:371:GLU:C	1:E:373:ILE:H	2.25	0.44
1:E:404:ARG:O	1:E:407:ALA:HB3	2.17	0.44
1:F:289:PHE:HA	1:F:325:GLN:HE21	1.82	0.44
1:F:331:THR:O	1:F:334:GLY:N	2.38	0.44
1:A:482:SER:OG	1:A:484:THR:OG1	2.32	0.44
1:B:289:PHE:N	1:B:296:ASN:HD21	2.09	0.44
1:C:492:LEU:C	1:C:494:GLN:H	2.26	0.44
1:C:524:THR:C	1:C:526:ASP:H	2.24	0.44
1:D:542:LEU:HD12	1:D:542:LEU:HA	1.81	0.44
1:F:442:ILE:HG21	1:F:488:GLY:CA	2.48	0.44
1:A:288:LEU:HB3	1:A:296:ASN:OD1	2.17	0.44
1:C:450:LYS:HD2	1:C:450:LYS:O	2.18	0.44
1:D:405:LEU:O	1:D:409:LEU:HG	2.17	0.44
1:F:437:ASP:C	1:F:439:ARG:H	2.26	0.44
1:A:287:LEU:HD11	1:A:335:LYS:HG3	1.99	0.44
1:A:368:LEU:HA	1:A:371:GLU:HG3	2.00	0.44
1:A:498:THR:HG23	1:A:520:LYS:O	2.18	0.44
1:B:515:LEU:C	1:B:515:LEU:HD23	2.42	0.44
1:C:289:PHE:H	1:C:296:ASN:HD21	1.65	0.44
1:C:411:TYR:CD1	1:C:415:GLY:HA3	2.53	0.44
1:D:367:SER:O	1:D:371:GLU:CG	2.66	0.44
1:D:466:LEU:CD2	1:D:486:LEU:HD23	2.47	0.44
1:A:385:LEU:HD23	1:A:386:PHE:CE2	2.53	0.43
1:A:405:LEU:HD11	1:A:409:LEU:HD21	1.99	0.43
1:A:515:LEU:C	1:A:515:LEU:CD2	2.89	0.43
1:B:393:LEU:HD12	1:B:393:LEU:H	1.79	0.43
1:C:275:ILE:O	1:C:278:HIS:HB3	2.18	0.43
1:C:309:MET:HB3	1:C:499:ILE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:ILE:O	1:E:279:LEU:HG	2.17	0.43
1:F:309:MET:HB3	1:F:499:ILE:HG12	2.00	0.43
1:A:401:GLU:HG2	1:A:402:THR:H	1.82	0.43
1:B:309:MET:HE1	1:B:462:VAL:HG12	2.00	0.43
1:C:331:THR:O	1:C:333:MET:N	2.51	0.43
1:E:367:SER:O	1:E:371:GLU:HG2	2.17	0.43
1:E:431:SER:HB3	1:E:441:MET:HE1	1.97	0.43
1:F:359:ARG:HB3	1:F:539:THR:HG22	2.00	0.43
1:F:449:LEU:O	1:F:452:PHE:HB3	2.18	0.43
1:B:371:GLU:C	1:B:373:ILE:H	2.25	0.43
1:C:478:GLY:O	1:C:479:ARG:O	2.36	0.43
1:D:482:SER:HG	1:D:484:THR:HG1	1.62	0.43
1:E:290:SER:N	1:E:325:GLN:HE21	2.05	0.43
1:E:379:ASP:OD2	1:F:276:ARG:NH2	2.51	0.43
1:E:388:ASN:O	1:E:389:ASP:C	2.61	0.43
1:F:311:THR:O	1:F:312:SER:HB3	2.18	0.43
1:F:467:LYS:O	1:F:469:PRO:HD3	2.18	0.43
1:B:316:MET:CE	1:B:504:ARG:H	2.29	0.43
1:B:403:ASP:O	1:B:407:ALA:HB2	2.18	0.43
1:C:282:GLU:OE1	1:C:282:GLU:HA	2.18	0.43
1:D:287:LEU:O	1:D:301:GLY:HA3	2.18	0.43
1:D:309:MET:O	1:D:500:ILE:N	2.49	0.43
1:D:405:LEU:HG	1:D:409:LEU:HD11	2.00	0.43
1:E:312:SER:OG	1:E:318:LYS:HG3	2.18	0.43
1:E:403:ASP:O	1:E:407:ALA:HB2	2.18	0.43
1:A:519:LEU:O	1:A:520:LYS:HB2	2.18	0.43
1:B:404:ARG:HG3	1:B:404:ARG:HH11	1.83	0.43
1:C:312:SER:OG	1:C:318:LYS:CG	2.67	0.43
1:C:492:LEU:O	1:C:494:GLN:N	2.51	0.43
1:D:439:ARG:O	1:D:443:ASP:OD2	2.36	0.43
1:E:309:MET:HE1	1:E:462:VAL:HG12	2.00	0.43
1:E:309:MET:O	1:E:500:ILE:N	2.41	0.43
1:F:413:ARG:CD	1:F:458:VAL:HB	2.47	0.43
1:F:498:THR:HA	1:F:520:LYS:O	2.19	0.43
1:A:394:TYR:OH	1:A:400:ALA:HB2	2.18	0.43
1:B:468:ASN:HD21	1:C:493:ARG:NE	2.15	0.43
1:C:505:ASN:HD22	1:C:507:GLN:H	1.66	0.43
1:E:518:ILE:HG22	1:E:518:ILE:O	2.19	0.43
1:F:327:LEU:HD13	1:F:353:LEU:CD2	2.40	0.43
1:A:367:SER:O	1:A:371:GLU:CG	2.67	0.43
1:A:426:ILE:HG22	1:A:464:CYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:SER:O	1:A:429:VAL:N	2.52	0.43
1:B:303:ARG:NH2	1:B:523:PHE:HB3	2.33	0.43
1:B:492:LEU:O	1:B:494:GLN:N	2.52	0.43
1:D:331:THR:HG22	1:D:332:ALA:N	2.33	0.43
1:D:401:GLU:HG2	1:D:402:THR:H	1.83	0.43
1:D:466:LEU:HB3	1:D:475:HIS:HE1	1.84	0.43
1:D:498:THR:HG22	1:D:499:ILE:N	2.33	0.43
1:E:404:ARG:HG3	1:E:404:ARG:HH11	1.82	0.43
1:E:409:LEU:HA	1:E:412:MET:HE2	2.01	0.43
1:E:515:LEU:C	1:E:515:LEU:HD23	2.43	0.43
1:F:303:ARG:NH2	1:F:523:PHE:CB	2.81	0.43
1:F:443:ASP:CG	1:F:491:ALA:HB2	2.43	0.43
1:C:307:VAL:HB	1:C:496:SER:HA	2.00	0.43
1:C:547:TYR:CG	1:C:548:SER:N	2.87	0.43
1:F:291:GLY:O	1:F:292:CYS:HB2	2.18	0.43
1:F:452:PHE:O	1:F:456:THR:OG1	2.34	0.43
1:A:407:ALA:O	1:A:410:ALA:HB3	2.18	0.43
1:B:458:VAL:HG22	1:B:459:VAL:N	2.34	0.43
1:D:283:GLU:O	1:D:303:ARG:CZ	2.67	0.43
1:D:333:MET:O	1:D:335:LYS:HG2	2.18	0.43
1:F:289:PHE:CA	1:F:325:GLN:HE21	2.32	0.43
1:F:450:LYS:HE2	1:F:454:LYS:HD2	2.01	0.43
1:F:492:LEU:C	1:F:494:GLN:H	2.26	0.43
1:A:424:ASP:OD1	1:A:424:ASP:C	2.62	0.43
1:A:439:ARG:O	1:A:443:ASP:OD2	2.37	0.43
1:A:480:PRO:HA	1:A:503:GLU:OE2	2.18	0.43
1:B:278:HIS:C	1:B:280:SER:H	2.27	0.43
1:B:547:TYR:CG	1:B:548:SER:N	2.86	0.43
1:C:296:ASN:HD22	1:C:296:ASN:HA	1.68	0.43
1:B:327:LEU:HD21	1:B:357:HIS:CA	2.47	0.42
1:D:363:ARG:C	1:D:365:SER:H	2.27	0.42
1:E:492:LEU:O	1:E:494:GLN:N	2.52	0.42
1:F:505:ASN:HD22	1:F:507:GLN:H	1.66	0.42
1:F:547:TYR:CG	1:F:548:SER:N	2.86	0.42
1:A:357:HIS:ND1	1:A:385:LEU:HB2	2.34	0.42
1:C:288:LEU:HB3	1:C:296:ASN:ND2	2.33	0.42
1:C:488:GLY:O	1:C:489:SER:C	2.61	0.42
1:D:283:GLU:HB2	1:D:523:PHE:CD2	2.53	0.42
1:E:375:ASN:HD21	1:E:377:LYS:CD	2.31	0.42
1:A:303:ARG:HB2	1:A:306:GLU:OE2	2.19	0.42
1:B:375:ASN:HD21	1:B:377:LYS:CD	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:GLU:HA	1:C:505:ASN:ND2	2.34	0.42
1:F:331:THR:O	1:F:333:MET:N	2.52	0.42
1:A:287:LEU:C	1:A:288:LEU:HD12	2.45	0.42
1:B:344:GLU:OE2	1:B:349:THR:HG22	2.19	0.42
1:C:443:ASP:CG	1:C:491:ALA:HB2	2.44	0.42
1:F:266:VAL:HG12	1:F:270:SER:OG	2.19	0.42
1:F:312:SER:OG	1:F:318:LYS:CG	2.66	0.42
1:B:506:GLN:HG2	1:B:506:GLN:H	1.61	0.42
1:E:458:VAL:HG22	1:E:459:VAL:N	2.34	0.42
1:E:547:TYR:CG	1:E:548:SER:N	2.87	0.42
1:F:267:SER:O	1:F:268:ALA:C	2.62	0.42
1:F:405:LEU:C	1:F:407:ALA:N	2.76	0.42
1:F:492:LEU:HD12	1:F:492:LEU:N	2.34	0.42
1:A:424:ASP:O	1:A:425:HIS:HB3	2.19	0.42
1:B:269:LEU:C	1:B:271:LEU:N	2.75	0.42
1:C:282:GLU:O	1:C:282:GLU:CG	2.66	0.42
1:C:299:THR:O	1:C:303:ARG:NH1	2.40	0.42
1:C:371:GLU:O	1:C:372:ILE:C	2.62	0.42
1:D:524:THR:C	1:D:526:ASP:N	2.64	0.42
1:E:387:GLY:C	1:E:389:ASP:H	2.28	0.42
1:F:368:LEU:HD23	1:F:368:LEU:HA	1.82	0.42
1:A:413:ARG:HD3	1:A:458:VAL:HB	2.00	0.42
1:B:312:SER:OG	1:B:318:LYS:HG3	2.19	0.42
1:C:287:LEU:HD21	1:C:420:VAL:HG21	2.01	0.42
1:C:439:ARG:O	1:C:442:ILE:HG22	2.20	0.42
1:C:466:LEU:HB3	1:C:475:HIS:HE1	1.85	0.42
1:D:425:HIS:CE1	1:D:427:SER:CB	2.93	0.42
1:E:518:ILE:CG2	1:E:527:THR:HA	2.50	0.42
1:F:371:GLU:O	1:F:372:ILE:C	2.62	0.42
1:F:401:GLU:HB3	1:F:404:ARG:CB	2.47	0.42
1:F:458:VAL:HG22	1:F:459:VAL:H	1.85	0.42
1:B:336:LYS:HB2	1:B:418:CYS:HA	2.02	0.42
1:C:411:TYR:CD1	1:C:411:TYR:C	2.95	0.42
1:C:442:ILE:HG21	1:C:488:GLY:CA	2.49	0.42
1:C:536:ASN:C	1:C:536:ASN:HD22	2.27	0.42
1:D:468:ASN:HA	1:D:469:PRO:HD2	1.84	0.42
1:E:312:SER:HB2	1:E:502:LEU:O	2.20	0.42
1:E:336:LYS:HB2	1:E:418:CYS:HA	2.02	0.42
1:E:425:HIS:H	1:E:463:ILE:HB	1.84	0.42
1:E:446:MET:O	1:E:449:LEU:N	2.53	0.42
1:F:492:LEU:O	1:F:494:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:LEU:CA	1:C:296:ASN:HD21	2.32	0.42
1:C:450:LYS:HE2	1:C:454:LYS:HD2	2.02	0.42
1:D:327:LEU:O	1:D:328:GLN:C	2.62	0.42
1:D:426:ILE:CG2	1:D:464:CYS:HB3	2.50	0.42
1:F:325:GLN:HB3	1:F:329:TRP:CZ3	2.55	0.42
1:A:289:PHE:CD2	1:A:295:ILE:HG22	2.55	0.42
1:A:303:ARG:NH2	1:A:523:PHE:HB2	2.35	0.42
1:E:393:LEU:HD12	1:E:393:LEU:H	1.79	0.42
1:F:362:LEU:O	1:F:369:LYS:HE2	2.20	0.42
1:A:372:ILE:HD13	1:A:381:TRP:HZ3	1.83	0.41
1:A:382:PHE:CZ	1:B:272:ARG:HB2	2.55	0.41
1:A:466:LEU:HB3	1:A:475:HIS:HE1	1.85	0.41
1:B:312:SER:HB2	1:B:502:LEU:O	2.20	0.41
1:C:309:MET:HB3	1:C:499:ILE:HG12	2.02	0.41
1:C:401:GLU:HB3	1:C:404:ARG:CB	2.47	0.41
1:D:309:MET:O	1:D:499:ILE:HA	2.19	0.41
1:D:513:LEU:HD12	1:D:533:MET:O	2.21	0.41
1:D:518:ILE:HD13	1:D:530:ALA:HB2	1.98	0.41
1:B:377:LYS:O	1:B:380:GLN:HB2	2.20	0.41
1:C:458:VAL:HG22	1:C:459:VAL:H	1.85	0.41
1:E:377:LYS:O	1:E:380:GLN:HB2	2.20	0.41
1:F:477:GLU:HA	1:F:505:ASN:ND2	2.35	0.41
1:D:427:SER:O	1:D:429:VAL:N	2.52	0.41
1:D:539:THR:OG1	1:D:541:TRP:HB2	2.20	0.41
1:E:345:SER:OG	1:E:347:GLU:HG2	2.20	0.41
1:F:267:SER:O	1:F:270:SER:OG	2.32	0.41
1:F:421:ILE:HB	1:F:460:LEU:HD12	2.01	0.41
1:F:463:ILE:HD13	1:F:463:ILE:HG21	1.87	0.41
1:A:405:LEU:O	1:A:409:LEU:HG	2.20	0.41
1:A:416:LEU:N	1:A:416:LEU:HD23	2.35	0.41
1:B:440:LYS:NZ	1:B:444:ASN:HB2	2.35	0.41
1:C:498:THR:HA	1:C:520:LYS:O	2.21	0.41
1:D:283:GLU:CG	1:D:523:PHE:CE2	3.03	0.41
1:D:340:ALA:H	1:D:341:MET:CE	2.32	0.41
1:D:416:LEU:HD23	1:D:416:LEU:N	2.35	0.41
1:D:515:LEU:HD21	1:D:517:ARG:HB2	2.03	0.41
1:F:276:ARG:O	1:F:277:GLU:C	2.63	0.41
1:F:437:ASP:C	1:F:439:ARG:N	2.79	0.41
1:A:446:MET:CG	1:A:492:LEU:HB3	2.45	0.41
1:D:286:GLY:O	1:D:287:LEU:O	2.39	0.41
1:D:289:PHE:N	1:D:296:ASN:HD21	2.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:PHE:CE1	1:E:275:ILE:HD12	2.55	0.41
1:E:506:GLN:HG2	1:E:506:GLN:H	1.61	0.41
1:A:287:LEU:O	1:A:301:GLY:HA3	2.20	0.41
1:B:348:GLU:O	1:B:351:GLU:HB3	2.20	0.41
1:C:271:LEU:O	1:C:272:ARG:C	2.63	0.41
1:C:401:GLU:OE1	1:C:404:ARG:N	2.50	0.41
1:C:452:PHE:O	1:C:456:THR:OG1	2.35	0.41
1:D:282:GLU:OE2	1:D:522:ARG:O	2.39	0.41
1:C:436:SER:O	1:C:437:ASP:O	2.39	0.41
1:C:468:ASN:HA	1:C:469:PRO:HD2	1.85	0.41
1:D:327:LEU:HA	1:D:327:LEU:HD12	1.83	0.41
1:D:343:GLU:HG3	1:D:428:ILE:CD1	2.50	0.41
1:E:373:ILE:HD11	1:F:279:LEU:CB	2.51	0.41
1:A:365:SER:OG	1:A:368:LEU:HB2	2.21	0.41
1:A:452:PHE:CE1	1:A:456:THR:HG21	2.55	0.41
1:C:437:ASP:C	1:C:439:ARG:N	2.78	0.41
1:C:518:ILE:O	1:C:518:ILE:HG22	2.20	0.41
1:C:537:LYS:HB3	1:C:537:LYS:HE2	1.77	0.41
1:E:479:ARG:HA	1:E:480:PRO:HD2	1.92	0.41
1:A:309:MET:O	1:A:499:ILE:HA	2.21	0.41
1:A:345:SER:OG	1:A:348:GLU:HG3	2.21	0.41
1:A:398:ALA:O	1:A:399:GLU:C	2.64	0.41
1:A:405:LEU:HG	1:A:409:LEU:HD11	2.03	0.41
1:B:287:LEU:HG	1:B:329:TRP:NE1	2.36	0.41
1:C:287:LEU:HG	1:C:329:TRP:NE1	2.36	0.41
1:C:311:THR:O	1:C:312:SER:HB3	2.21	0.41
1:C:324:GLN:HE22	1:C:542:LEU:HB2	1.85	0.41
1:C:325:GLN:HB3	1:C:329:TRP:CZ3	2.56	0.41
1:D:424:ASP:OD1	1:D:425:HIS:N	2.54	0.41
1:D:516:VAL:CG2	1:D:533:MET:HE2	2.51	0.41
1:E:359:ARG:HD3	1:E:541:TRP:NE1	2.35	0.41
1:E:369:LYS:NZ	1:F:282:GLU:HG3	2.36	0.41
1:F:289:PHE:HB3	1:F:325:GLN:NE2	2.36	0.41
1:F:406:LEU:O	1:F:410:ALA:HB2	2.20	0.41
1:A:340:ALA:H	1:A:341:MET:CE	2.34	0.41
1:C:413:ARG:CD	1:C:458:VAL:HB	2.51	0.41
1:E:437:ASP:C	1:E:439:ARG:H	2.29	0.41
1:C:411:TYR:O	1:C:415:GLY:N	2.51	0.40
1:D:445:LEU:HA	1:D:448:LYS:HE3	2.03	0.40
1:E:344:GLU:OE2	1:E:349:THR:HG22	2.20	0.40
1:F:468:ASN:HA	1:F:469:PRO:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ARG:C	1:A:365:SER:H	2.29	0.40
1:D:303:ARG:N	1:D:303:ARG:HD3	2.36	0.40
1:E:361:ARG:NH1	1:E:535:TYR:OH	2.54	0.40
1:A:324:GLN:HE22	1:A:542:LEU:HB2	1.86	0.40
1:B:388:ASN:O	1:B:389:ASP:C	2.63	0.40
1:D:424:ASP:O	1:D:425:HIS:HB3	2.21	0.40
1:F:358:ASN:C	1:F:360:VAL:HG22	2.46	0.40
1:F:404:ARG:NH1	1:F:408:LYS:CE	2.72	0.40
1:F:516:VAL:CG2	1:F:533:MET:HE3	2.51	0.40
1:B:387:GLY:C	1:B:389:ASP:H	2.28	0.40
1:B:519:LEU:HA	1:B:519:LEU:HD12	1.78	0.40
1:E:310:VAL:HG22	1:E:500:ILE:HB	2.04	0.40
1:F:340:ALA:HB3	1:F:423:LEU:HA	2.02	0.40
1:F:488:GLY:O	1:F:489:SER:C	2.62	0.40
1:B:502:LEU:HD23	1:B:514:VAL:HG21	2.02	0.40
1:C:407:ALA:O	1:C:410:ALA:HB3	2.21	0.40
1:D:474:ALA:O	1:D:476:GLU:N	2.54	0.40
1:E:307:VAL:N	1:E:497:ASP:OD2	2.39	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	284/289 (98%)	225 (79%)	34 (12%)	25 (9%)	0	4
1	B	286/289 (99%)	226 (79%)	42 (15%)	18 (6%)	1	8
1	C	286/289 (99%)	225 (79%)	45 (16%)	16 (6%)	1	9
1	D	284/289 (98%)	223 (78%)	34 (12%)	27 (10%)	0	3
1	E	286/289 (99%)	231 (81%)	37 (13%)	18 (6%)	1	8
1	F	286/289 (99%)	225 (79%)	40 (14%)	21 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1712/1734 (99%)	1355 (79%)	232 (14%)	125 (7%)	1	6

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	SER
1	A	436	SER
1	A	437	ASP
1	A	475	HIS
1	A	489	SER
1	A	490	GLY
1	B	279	LEU
1	B	371	GLU
1	B	372	ILE
1	B	396	SER
1	B	399	GLU
1	B	432	ALA
1	B	436	SER
1	B	437	ASP
1	B	475	HIS
1	B	490	GLY
1	C	292	CYS
1	C	371	GLU
1	C	436	SER
1	C	437	ASP
1	C	475	HIS
1	C	479	ARG
1	C	490	GLY
1	D	281	SER
1	D	396	SER
1	D	436	SER
1	D	437	ASP
1	D	475	HIS
1	D	489	SER
1	D	490	GLY
1	E	371	GLU
1	E	372	ILE
1	E	396	SER
1	E	399	GLU
1	E	432	ALA
1	E	436	SER
1	E	437	ASP

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Mol	Chain	Res	Type
1	E	475	HIS
1	E	490	GLY
1	F	371	GLU
1	F	436	SER
1	F	437	ASP
1	F	475	HIS
1	F	479	ARG
1	F	490	GLY
1	A	399	GLU
1	A	432	ALA
1	A	438	GLU
1	A	525	GLY
1	A	537	LYS
1	B	334	GLY
1	C	332	ALA
1	C	372	ILE
1	C	396	SER
1	C	399	GLU
1	C	432	ALA
1	C	488	GLY
1	C	522	ARG
1	D	272	ARG
1	D	287	LEU
1	D	371	GLU
1	D	399	GLU
1	D	432	ALA
1	D	438	GLU
1	D	525	GLY
1	D	537	LYS
1	E	334	GLY
1	E	388	ASN
1	F	292	CYS
1	F	332	ALA
1	F	372	ILE
1	F	396	SER
1	F	399	GLU
1	F	432	ALA
1	A	281	SER
1	A	371	GLU
1	A	485	ASP
1	B	388	ASN
1	B	397	PHE

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Mol	Chain	Res	Type
1	B	479	ARG
1	C	397	PHE
1	C	406	LEU
1	D	271	LEU
1	D	285	VAL
1	D	485	ASP
1	E	479	ARG
1	E	537	LYS
1	F	269	LEU
1	F	279	LEU
1	F	281	SER
1	F	287	LEU
1	F	397	PHE
1	F	406	LEU
1	F	488	GLY
1	F	522	ARG
1	A	334	GLY
1	A	397	PHE
1	A	479	ARG
1	A	487	ARG
1	A	548	SER
1	B	318	LYS
1	B	471	LYS
1	B	537	LYS
1	D	397	PHE
1	D	479	ARG
1	D	487	ARG
1	D	548	SER
1	E	318	LYS
1	E	397	PHE
1	E	471	LYS
1	A	327	LEU
1	A	471	LYS
1	A	523	PHE
1	D	334	GLY
1	D	471	LYS
1	E	292	CYS
1	E	389	ASP
1	F	278	HIS
1	A	287	LEU
1	D	523	PHE
1	B	264	GLY

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Mol	Chain	Res	Type
1	A	428	ILE
1	A	488	GLY
1	D	428	ILE
1	D	488	GLY

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	241/242 (100%)	208 (86%)	33 (14%)	3	16
1	B	241/242 (100%)	214 (89%)	27 (11%)	6	22
1	C	241/242 (100%)	214 (89%)	27 (11%)	6	22
1	D	241/242 (100%)	210 (87%)	31 (13%)	4	17
1	E	241/242 (100%)	212 (88%)	29 (12%)	5	20
1	F	241/242 (100%)	216 (90%)	25 (10%)	7	25
All	All	1446/1452 (100%)	1274 (88%)	172 (12%)	5	20

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	ARG
1	A	277	GLU
1	A	288	LEU
1	A	314	SER
1	A	322	VAL
1	A	324	GLN
1	A	328	GLN
1	A	342	LEU
1	A	347	GLU
1	A	349	THR
1	A	360	VAL
1	A	368	LEU
1	A	373	ILE
1	A	375	ASN

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Mol	Chain	Res	Type
1	A	384	GLU
1	A	393	LEU
1	A	403	ASP
1	A	406	LEU
1	A	446	MET
1	A	470	ASP
1	A	476	GLU
1	A	481	VAL
1	A	487	ARG
1	A	492	LEU
1	A	495	LEU
1	A	506	GLN
1	A	507	GLN
1	A	512	ASN
1	A	515	LEU
1	A	518	ILE
1	A	522	ARG
1	A	524	THR
1	A	542	LEU
1	B	277	GLU
1	B	290	SER
1	B	347	GLU
1	B	349	THR
1	B	360	VAL
1	B	368	LEU
1	B	373	ILE
1	B	384	GLU
1	B	393	LEU
1	B	394	TYR
1	B	420	VAL
1	B	440	LYS
1	B	468	ASN
1	B	470	ASP
1	B	476	GLU
1	B	477	GLU
1	B	481	VAL
1	B	487	ARG
1	B	492	LEU
1	B	493	ARG
1	B	495	LEU
1	B	505	ASN
1	B	506	GLN

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Mol	Chain	Res	Type
1	B	507	GLN
1	B	512	ASN
1	B	515	LEU
1	B	519	LEU
1	C	266	VAL
1	C	273	GLU
1	C	274	ARG
1	C	283	GLU
1	C	287	LEU
1	C	314	SER
1	C	347	GLU
1	C	349	THR
1	C	360	VAL
1	C	368	LEU
1	C	384	GLU
1	C	390	THR
1	C	393	LEU
1	C	403	ASP
1	C	440	LYS
1	C	470	ASP
1	C	476	GLU
1	C	481	VAL
1	C	487	ARG
1	C	492	LEU
1	C	493	ARG
1	C	495	LEU
1	C	504	ARG
1	C	507	GLN
1	C	512	ASN
1	C	519	LEU
1	C	542	LEU
1	D	270	SER
1	D	277	GLU
1	D	314	SER
1	D	322	VAL
1	D	324	GLN
1	D	328	GLN
1	D	347	GLU
1	D	349	THR
1	D	360	VAL
1	D	368	LEU
1	D	373	ILE

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Mol	Chain	Res	Type
1	D	375	ASN
1	D	384	GLU
1	D	393	LEU
1	D	403	ASP
1	D	406	LEU
1	D	446	MET
1	D	470	ASP
1	D	476	GLU
1	D	481	VAL
1	D	487	ARG
1	D	492	LEU
1	D	495	LEU
1	D	506	GLN
1	D	507	GLN
1	D	512	ASN
1	D	515	LEU
1	D	518	ILE
1	D	522	ARG
1	D	524	THR
1	D	542	LEU
1	E	274	ARG
1	E	277	GLU
1	E	283	GLU
1	E	284	SER
1	E	290	SER
1	E	347	GLU
1	E	349	THR
1	E	360	VAL
1	E	368	LEU
1	E	373	ILE
1	E	384	GLU
1	E	393	LEU
1	E	394	TYR
1	E	420	VAL
1	E	440	LYS
1	E	468	ASN
1	E	470	ASP
1	E	476	GLU
1	E	477	GLU
1	E	481	VAL
1	E	487	ARG
1	E	492	LEU

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Mol	Chain	Res	Type
1	E	493	ARG
1	E	495	LEU
1	E	505	ASN
1	E	506	GLN
1	E	507	GLN
1	E	512	ASN
1	E	519	LEU
1	F	277	GLU
1	F	281	SER
1	F	283	GLU
1	F	287	LEU
1	F	347	GLU
1	F	349	THR
1	F	360	VAL
1	F	368	LEU
1	F	384	GLU
1	F	390	THR
1	F	393	LEU
1	F	403	ASP
1	F	440	LYS
1	F	470	ASP
1	F	476	GLU
1	F	481	VAL
1	F	487	ARG
1	F	492	LEU
1	F	493	ARG
1	F	495	LEU
1	F	504	ARG
1	F	507	GLN
1	F	512	ASN
1	F	519	LEU
1	F	542	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	324	GLN
1	A	325	GLN
1	A	358	ASN
1	A	375	ASN
1	A	392	HIS

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Mol	Chain	Res	Type
1	A	425	HIS
1	A	475	HIS
1	A	494	GLN
1	A	506	GLN
1	A	507	GLN
1	A	536	ASN
1	B	296	ASN
1	B	324	GLN
1	B	325	GLN
1	B	358	ASN
1	B	375	ASN
1	B	392	HIS
1	B	444	ASN
1	B	505	ASN
1	B	507	GLN
1	B	536	ASN
1	C	296	ASN
1	C	324	GLN
1	C	325	GLN
1	C	358	ASN
1	C	375	ASN
1	C	392	HIS
1	C	468	ASN
1	C	475	HIS
1	C	494	GLN
1	C	505	ASN
1	C	536	ASN
1	D	296	ASN
1	D	325	GLN
1	D	358	ASN
1	D	375	ASN
1	D	380	GLN
1	D	425	HIS
1	D	475	HIS
1	D	494	GLN
1	D	507	GLN
1	D	536	ASN
1	E	296	ASN
1	E	324	GLN
1	E	325	GLN
1	E	358	ASN
1	E	375	ASN

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Mol	Chain	Res	Type
1	E	444	ASN
1	E	494	GLN
1	E	505	ASN
1	E	536	ASN
1	F	324	GLN
1	F	325	GLN
1	F	358	ASN
1	F	375	ASN
1	F	392	HIS
1	F	468	ASN
1	F	475	HIS
1	F	494	GLN
1	F	505	ASN
1	F	536	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	283:GLU	C	284:SER	N	7.79
1	A	283:GLU	C	284:SER	N	6.86

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	288/289 (99%)	-0.30	2 (0%) 84 70	40, 88, 175, 200	0
1	B	288/289 (99%)	-0.38	1 (0%) 90 82	23, 71, 167, 200	0
1	C	288/289 (99%)	-0.39	1 (0%) 90 82	30, 73, 168, 192	0
1	D	288/289 (99%)	-0.05	1 (0%) 90 82	65, 117, 178, 200	0
1	E	288/289 (99%)	-0.22	1 (0%) 90 82	47, 103, 176, 200	0
1	F	288/289 (99%)	-0.32	1 (0%) 90 82	43, 94, 172, 200	0
All	All	1728/1734 (99%)	-0.28	7 (0%) 88 79	23, 92, 175, 200	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	399	GLU	3.2
1	F	293	THR	2.6
1	B	436	SER	2.4
1	A	430	VAL	2.4
1	D	526	ASP	2.4
1	A	305	GLY	2.3
1	C	436	SER	2.1

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.