



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:15 AM UTC

PDB ID : 1WP9 / pdb_00001wp9
Title : Crystal structure of Pyrococcus furiosus Hef helicase domain
Authors : Nishino, T.; Komori, K.; Tsuchiya, D.; Ishino, Y.; Morikawa, K.
Deposited on : 2004-08-31
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

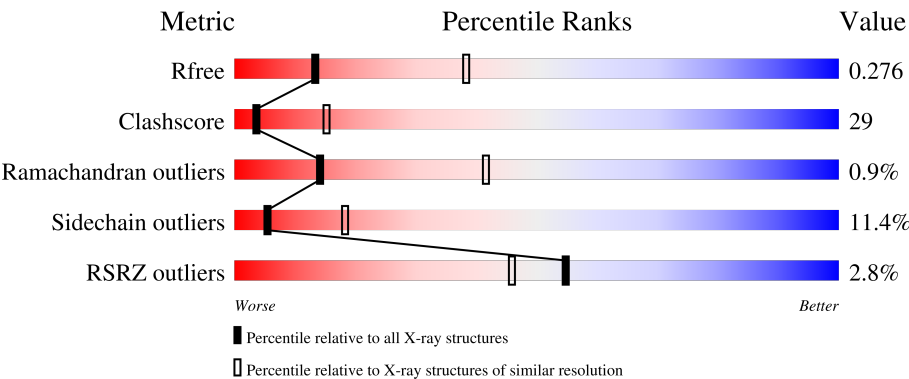
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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	494	4% 49%39%9% .
1	B	494	3% 48%40%7% .
1	C	494	4% 44%43%9% .
1	D	494	3% 47%40%7%5%
1	E	494	% 46%43%7% .

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Mol	Chain	Length	Quality of chain
1	F	494	% 45% 43% 8% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	495	-	-	X	-
2	PO4	C	495	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22913 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 ATP-dependent RNA helicase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3831	2445	683	689	14			
1	B	477	Total	C	N	O	S	0	0	0
			3817	2436	680	687	14			
1	C	475	Total	C	N	O	S	0	0	0
			3807	2431	678	684	14			
1	D	469	Total	C	N	O	S	0	0	0
			3765	2407	670	674	14			
1	E	475	Total	C	N	O	S	0	0	0
			3807	2431	678	684	14			
1	F	475	Total	C	N	O	S	0	0	0
			3807	2431	678	684	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP Q8TZH8
B	2	VAL	LEU	engineered mutation	UNP Q8TZH8
C	2	VAL	LEU	engineered mutation	UNP Q8TZH8
D	2	VAL	LEU	engineered mutation	UNP Q8TZH8
E	2	VAL	LEU	engineered mutation	UNP Q8TZH8
F	2	VAL	LEU	engineered mutation	UNP Q8TZH8

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

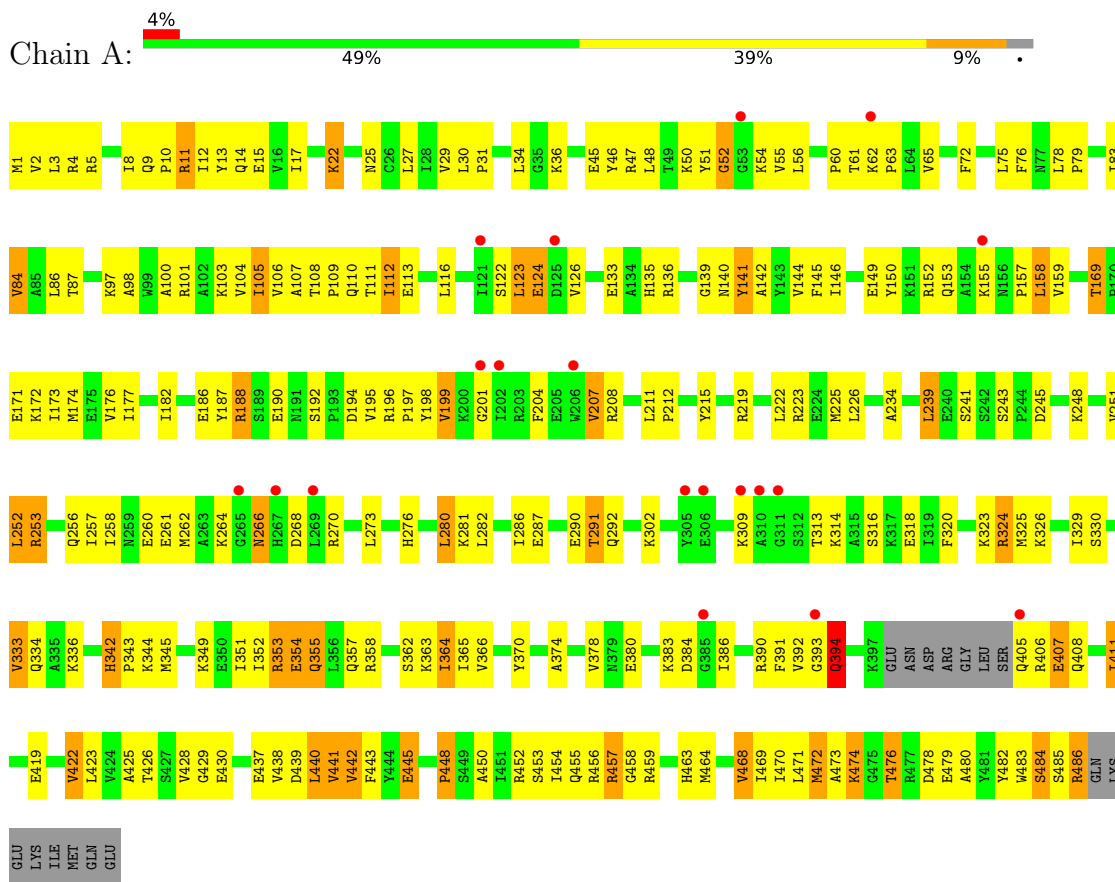
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	13	Total	O	0	0
			13	13		
3	C	8	Total	O	0	0
			8	8		
3	D	7	Total	O	0	0
			7	7		
3	E	13	Total	O	0	0
			13	13		
3	F	4	Total	O	0	0
			4	4		

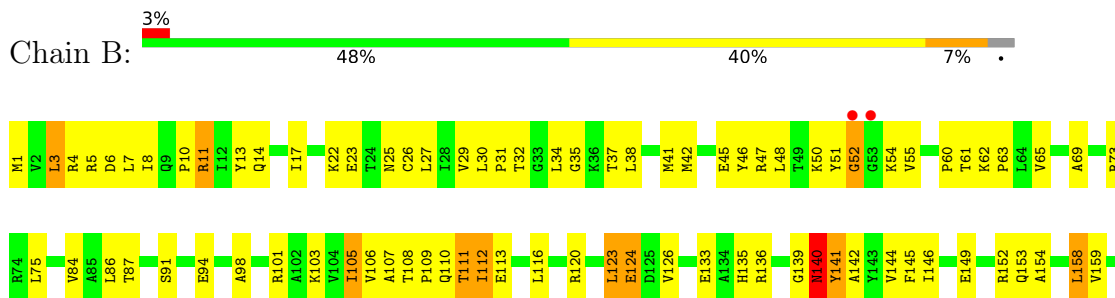
3 Residue-property plots

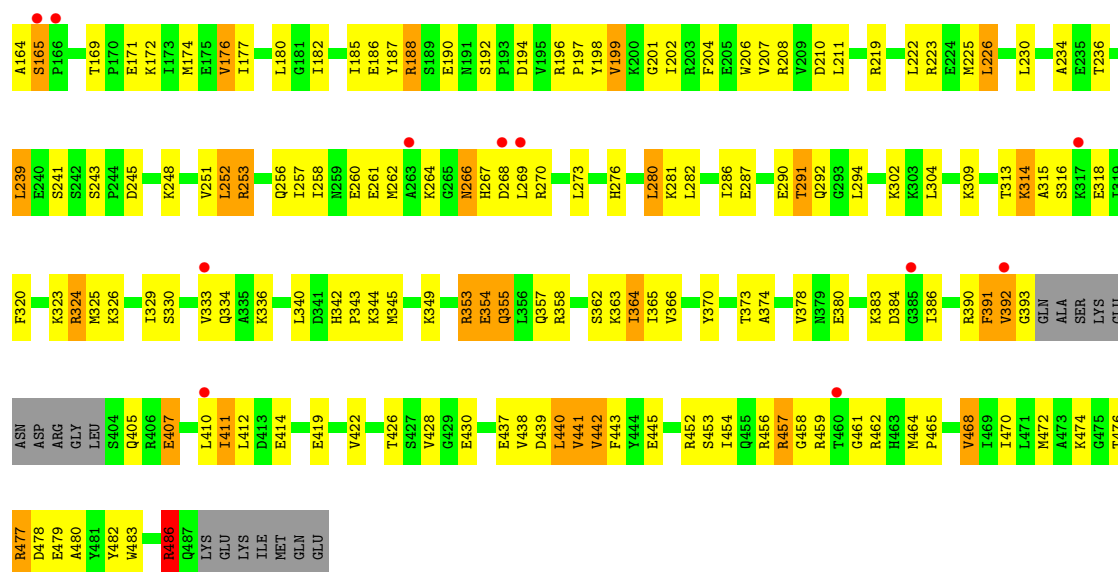
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

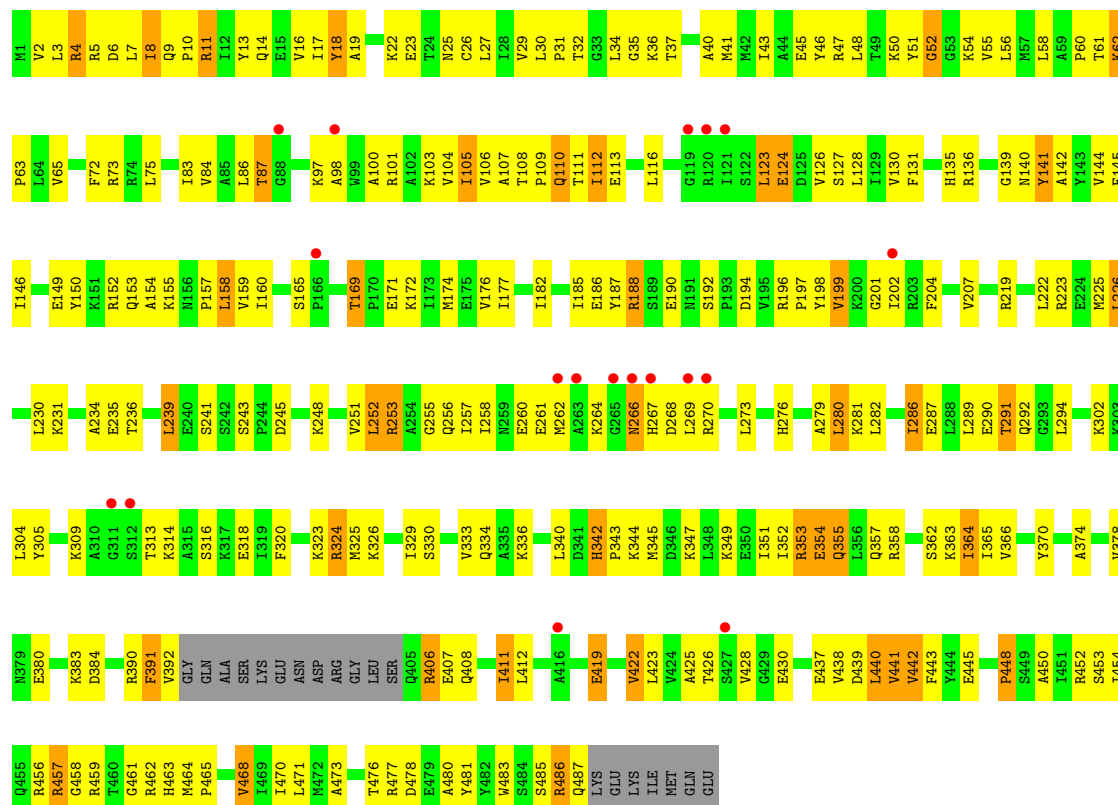
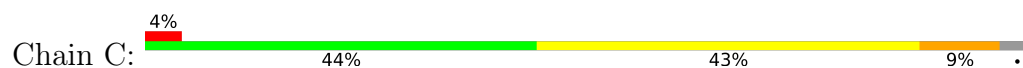


- Molecule 1: ATP-dependent RNA helicase, putative



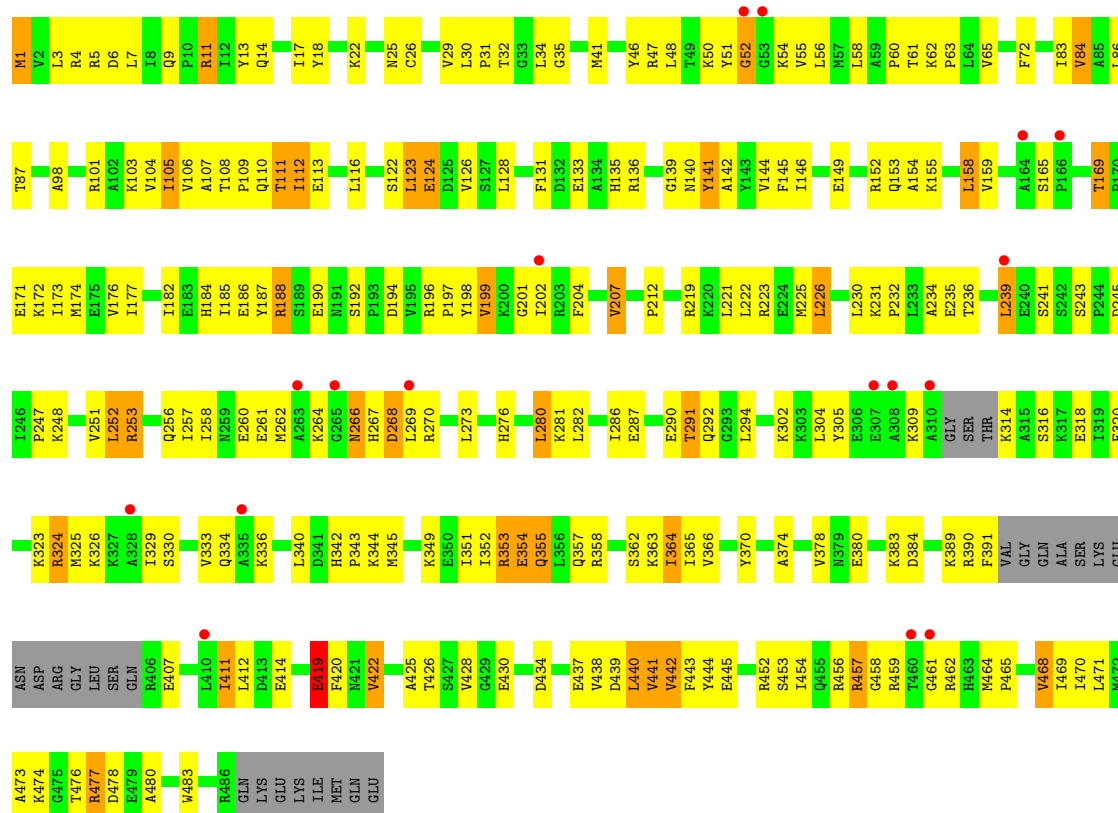


- Molecule 1: ATP-dependent RNA helicase, putative

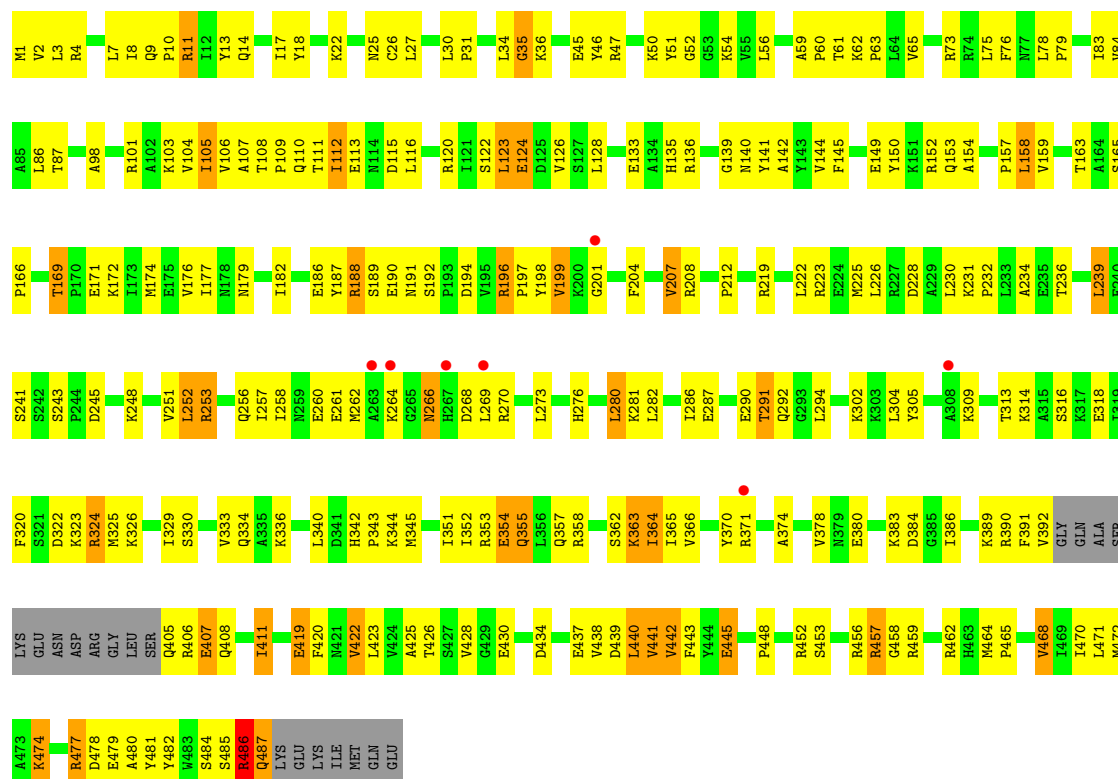


- Molecule 1: ATP-dependent RNA helicase, putative

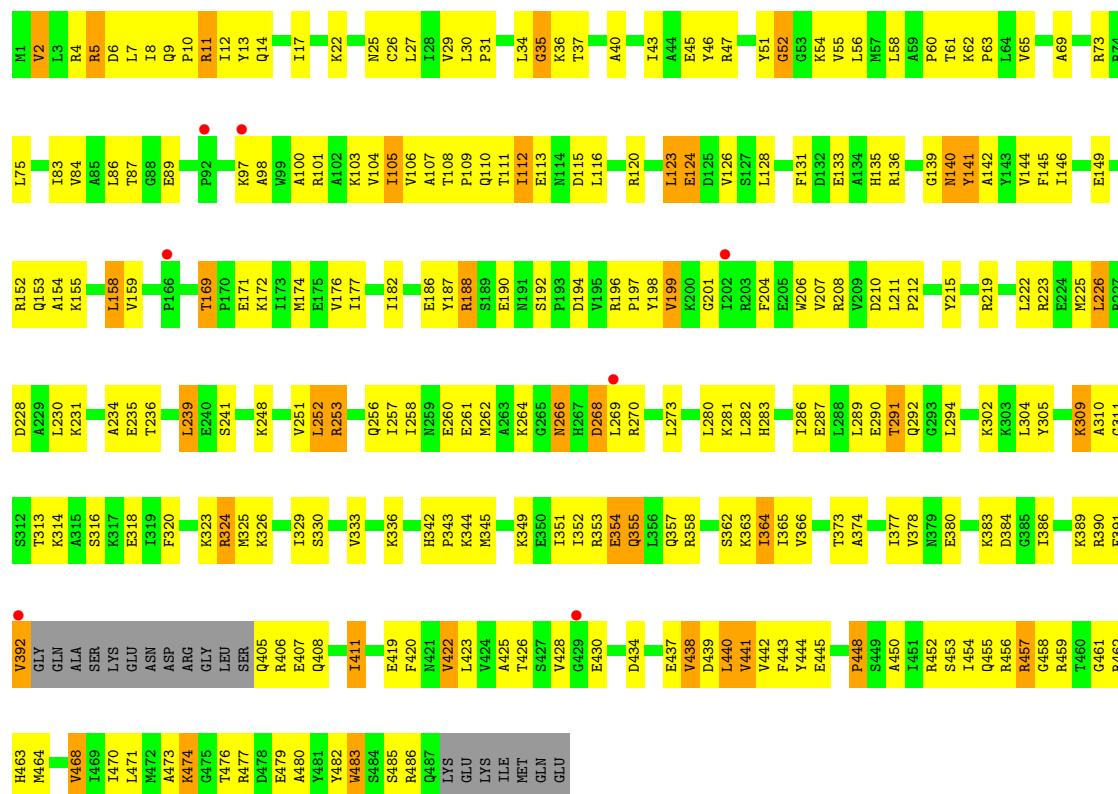




- Molecule 1: ATP-dependent RNA helicase, putative



Chain F: 45% 43% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.50Å 165.94Å 119.16Å 90.00° 114.85° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (15.00-2.90) 96.4 (15.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.76Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.286 0.249 , 0.276	Depositor DCC
R_{free} test set	9383 reflections (9.05%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22913	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.57	0/3894	1.00	14/5241 (0.3%)
1	B	0.57	0/3880	1.02	17/5223 (0.3%)
1	C	0.54	0/3870	1.01	13/5210 (0.2%)
1	D	0.52	0/3827	0.99	11/5150 (0.2%)
1	E	0.55	0/3870	1.02	16/5210 (0.3%)
1	F	0.52	0/3870	1.01	14/5210 (0.3%)
All	All	0.55	0/23211	1.01	85/31244 (0.3%)

There are no bond length outliers.

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	ARG	NE-CZ-NH2	7.60	126.04	119.20
1	E	439	ASP	N-CA-C	7.48	119.43	111.28
1	C	35	GLY	N-CA-C	7.39	125.57	115.30
1	E	196	ARG	NE-CZ-NH2	7.28	125.75	119.20
1	A	439	ASP	N-CA-C	7.24	119.17	111.28
1	E	196	ARG	NE-CZ-NH1	-7.19	114.31	121.50
1	C	439	ASP	N-CA-C	7.16	118.74	111.07
1	D	439	ASP	N-CA-C	7.16	119.70	111.11
1	F	201	GLY	N-CA-C	-7.15	102.91	112.14
1	B	439	ASP	N-CA-C	7.04	119.56	111.11
1	F	439	ASP	N-CA-C	6.96	119.75	111.33
1	E	384	ASP	N-CA-C	-6.92	99.14	109.86
1	D	201	GLY	N-CA-C	-6.90	102.15	111.54
1	B	407	GLU	N-CA-C	-6.74	103.74	112.23
1	B	120	ARG	NE-CZ-NH1	-6.73	114.77	121.50
1	F	35	GLY	N-CA-C	6.58	124.70	115.43
1	F	384	ASP	N-CA-C	-6.55	99.57	109.79
1	B	477	ARG	N-CA-C	-6.53	105.17	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	HIS	CA-C-N	6.49	127.00	119.47
1	A	342	HIS	C-N-CA	6.49	127.00	119.47
1	A	384	ASP	N-CA-C	-6.47	99.70	109.79
1	D	35	GLY	N-CA-C	6.42	124.48	115.43
1	C	445	GLU	N-CA-C	-6.39	100.83	108.25
1	C	201	GLY	N-CA-C	-6.29	104.03	112.14
1	C	384	ASP	N-CA-C	-6.27	100.01	109.79
1	F	486	ARG	N-CA-C	-6.24	105.24	112.92
1	E	486	ARG	N-CA-C	-6.24	104.76	113.37
1	D	103	LYS	N-CA-C	-6.21	106.02	113.97
1	C	342	HIS	CA-C-N	6.16	126.06	119.28
1	C	342	HIS	C-N-CA	6.16	126.06	119.28
1	F	103	LYS	N-CA-C	-6.14	106.11	113.97
1	E	201	GLY	N-CA-C	-6.14	104.22	112.14
1	A	201	GLY	N-CA-C	-6.13	104.23	112.14
1	C	103	LYS	N-CA-C	-6.00	106.28	113.97
1	A	407	GLU	N-CA-C	-6.00	104.81	111.71
1	B	384	ASP	N-CA-C	-5.94	100.52	109.79
1	B	35	GLY	N-CA-C	5.88	124.02	115.32
1	D	384	ASP	N-CA-C	-5.87	100.63	109.79
1	A	422	VAL	N-CA-C	5.86	116.31	108.11
1	D	26	CYS	N-CA-C	5.84	118.58	109.52
1	E	445	GLU	N-CA-C	-5.79	101.49	108.14
1	A	445	GLU	N-CA-C	-5.76	101.52	108.14
1	A	386	ILE	N-CA-C	5.75	116.75	108.48
1	B	103	LYS	N-CA-C	-5.73	106.64	113.97
1	B	314	LYS	N-CA-C	-5.72	105.03	112.23
1	B	201	GLY	N-CA-C	-5.69	103.81	111.54
1	E	422	VAL	N-CA-C	5.68	116.06	108.11
1	D	445	GLU	N-CA-C	-5.65	101.70	108.25
1	B	26	CYS	N-CA-C	5.62	118.23	109.52
1	C	26	CYS	N-CA-C	5.59	117.91	109.41
1	D	84	VAL	N-CA-C	5.58	116.63	108.53
1	F	386	ILE	N-CA-C	5.54	116.46	108.48
1	F	362	SER	N-CA-C	5.53	118.03	110.24
1	F	140	ASN	N-CA-C	5.48	118.43	111.69
1	A	195	VAL	N-CA-C	5.46	116.51	111.81
1	F	483	TRP	N-CA-C	-5.44	106.31	113.12
1	F	422	VAL	N-CA-C	5.43	115.71	108.11
1	B	445	GLU	N-CA-C	-5.42	101.97	108.25
1	E	362	SER	N-CA-C	5.42	117.88	110.24
1	D	422	VAL	N-CA-C	5.39	115.65	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	LYS	N-CA-C	-5.38	106.72	113.72
1	B	386	ILE	N-CA-C	5.35	116.19	108.48
1	F	26	CYS	N-CA-C	5.34	117.53	109.41
1	B	120	ARG	CD-NE-CZ	5.33	131.85	124.40
1	D	362	SER	N-CA-C	5.32	117.74	110.24
1	A	103	LYS	N-CA-C	-5.31	106.82	113.72
1	E	35	GLY	N-CA-C	5.24	123.30	115.64
1	C	286	ILE	CB-CA-C	-5.22	105.28	111.97
1	B	486	ARG	N-CA-C	-5.22	107.43	112.97
1	A	84	VAL	N-CA-C	5.22	116.82	108.89
1	A	362	SER	N-CA-C	5.21	117.59	110.24
1	E	26	CYS	N-CA-C	5.19	117.56	109.52
1	C	279	ALA	N-CA-C	-5.18	105.32	110.97
1	E	59	ALA	CA-C-N	5.16	126.29	119.84
1	E	59	ALA	C-N-CA	5.16	126.29	119.84
1	B	140	ASN	N-CA-C	5.15	118.02	111.69
1	E	196	ARG	CD-NE-CZ	5.13	131.59	124.40
1	A	333	VAL	N-CA-C	-5.12	106.15	111.58
1	F	268	ASP	N-CA-C	-5.08	105.20	111.40
1	F	310	ALA	N-CA-C	-5.08	106.19	112.38
1	C	422	VAL	N-CA-C	5.05	115.19	108.11
1	C	362	SER	N-CA-C	5.02	117.32	110.24
1	E	386	ILE	N-CA-C	5.02	115.71	108.48
1	D	268	ASP	N-CA-C	-5.02	105.28	111.40
1	B	362	SER	N-CA-C	5.01	117.30	110.24

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	3831	0	4023	244	0
1	B	3817	0	4005	227	1
1	C	3807	0	3997	252	0
1	D	3765	0	3956	242	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3807	0	3997	235	1
1	F	3807	0	3997	250	0
2	A	5	0	0	5	0
2	B	5	0	0	1	0
2	C	5	0	0	2	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
3	A	4	0	0	0	0
3	B	13	0	0	0	0
3	C	8	0	0	0	0
3	D	7	0	0	2	0
3	E	13	0	0	0	0
3	F	4	0	0	0	0
All	All	22913	0	23975	1372	1

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 29.

All (1372) 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:F:211:LEU:H	1:F:474:LYS:HE2	1.19	1.06
1:E:405:GLN:HB2	1:E:408:GLN:HG3	1.38	1.00
1:D:123:LEU:HD23	1:D:123:LEU:H	1.25	1.00
1:A:174:MET:HE3	1:E:480:ALA:HB2	1.43	0.98
1:E:426:THR:HG23	1:E:428:VAL:HG12	1.47	0.97
1:C:476:THR:HG23	1:C:478:ASP:H	1.27	0.97
1:F:426:THR:HG23	1:F:428:VAL:HG12	1.44	0.96
1:C:241:SER:HB2	1:D:139:GLY:HA2	1.45	0.95
1:F:169:THR:HG22	1:F:172:LYS:H	1.30	0.95
1:B:8:ILE:HD11	1:B:75:LEU:HD13	1.47	0.95
1:A:123:LEU:H	1:A:123:LEU:HD23	1.29	0.95
1:C:426:THR:HG23	1:C:428:VAL:HG12	1.48	0.95
1:E:123:LEU:HD23	1:E:123:LEU:H	1.32	0.94
1:D:426:THR:HG23	1:D:428:VAL:HG12	1.47	0.94
1:B:211:LEU:H	1:B:474:LYS:HE3	1.32	0.93
1:B:123:LEU:HD23	1:B:123:LEU:H	1.34	0.93
1:C:139:GLY:HA2	1:D:241:SER:CB	1.99	0.92
1:E:208:ARG:HD3	1:E:474:LYS:HG2	1.48	0.92
1:A:480:ALA:HB2	1:E:174:MET:HE3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:GLU:OE1	1:E:459:ARG:HD2	1.70	0.92
1:F:123:LEU:H	1:F:123:LEU:HD23	1.34	0.91
1:A:426:THR:HG23	1:A:428:VAL:HG12	1.52	0.91
1:E:477:ARG:HB3	1:E:477:ARG:NH1	1.84	0.91
1:A:65:VAL:HG13	1:A:106:VAL:HG12	1.50	0.91
1:F:65:VAL:HG13	1:F:106:VAL:HG12	1.53	0.90
1:C:65:VAL:HG13	1:C:106:VAL:HG12	1.53	0.90
1:E:472:MET:HE2	1:E:479:GLU:HA	1.50	0.90
1:D:378:VAL:HG21	1:D:390:ARG:HB2	1.54	0.89
1:B:426:THR:HG23	1:B:428:VAL:HG12	1.54	0.88
1:B:65:VAL:HG13	1:B:106:VAL:HG12	1.54	0.88
1:E:342:HIS:HD2	1:E:344:LYS:H	1.21	0.88
1:A:36:LYS:HE3	2:A:495:PO4:O2	1.74	0.88
1:F:473:ALA:O	1:F:476:THR:HG22	1.72	0.87
1:C:123:LEU:H	1:C:123:LEU:HD23	1.39	0.86
1:A:9:GLN:HE22	1:B:14:GLN:HE22	1.22	0.86
1:C:139:GLY:HA2	1:D:241:SER:HB3	1.58	0.86
1:F:11:ARG:H	1:F:14:GLN:HE21	1.24	0.85
1:B:378:VAL:HG21	1:B:390:ARG:HB2	1.60	0.84
1:E:116:LEU:HD11	1:E:123:LEU:HD22	1.56	0.84
1:D:473:ALA:O	1:D:476:THR:HG22	1.77	0.84
1:C:378:VAL:HG21	1:C:390:ARG:HB2	1.59	0.84
1:A:486:ARG:HH22	1:E:166:PRO:HD2	1.43	0.84
1:D:65:VAL:HG13	1:D:106:VAL:HG12	1.56	0.83
1:D:458:GLY:HA2	1:D:464:MET:HE1	1.60	0.83
1:E:208:ARG:CD	1:E:474:LYS:HG2	2.07	0.83
1:A:330:SER:O	1:A:333:VAL:HG12	1.79	0.83
1:E:391:PHE:HB2	1:E:423:LEU:HD11	1.60	0.83
1:F:11:ARG:H	1:F:14:GLN:NE2	1.75	0.83
1:E:208:ARG:HD3	1:E:474:LYS:CG	2.08	0.83
1:A:141:TYR:O	1:A:144:VAL:HG12	1.78	0.83
1:B:116:LEU:HD11	1:B:123:LEU:HD22	1.60	0.82
1:D:11:ARG:H	1:D:14:GLN:NE2	1.77	0.82
1:D:476:THR:HG23	1:D:478:ASP:H	1.44	0.82
1:D:477:ARG:NH1	1:D:477:ARG:HB3	1.94	0.82
1:F:116:LEU:HD11	1:F:123:LEU:HD22	1.62	0.82
1:D:141:TYR:O	1:D:144:VAL:HG12	1.79	0.81
1:B:141:TYR:O	1:B:144:VAL:HG12	1.79	0.81
1:C:458:GLY:HA2	1:C:464:MET:HE1	1.61	0.81
1:A:169:THR:HG22	1:A:172:LYS:H	1.46	0.81
1:F:378:VAL:HG21	1:F:390:ARG:HB2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ARG:O	1:A:486:ARG:HG2	1.80	0.81
1:B:241:SER:HB2	1:F:139:GLY:HA2	1.62	0.80
1:C:116:LEU:HD11	1:C:123:LEU:HD22	1.61	0.80
1:C:258:ILE:HG21	1:C:273:LEU:HD13	1.63	0.80
1:F:458:GLY:HA2	1:F:464:MET:HE1	1.63	0.80
1:C:169:THR:HG22	1:C:172:LYS:H	1.47	0.80
1:C:406:ARG:H	1:C:406:ARG:HD3	1.47	0.80
1:E:141:TYR:O	1:E:144:VAL:HG12	1.80	0.80
1:D:116:LEU:HD11	1:D:123:LEU:HD22	1.62	0.80
1:D:444:TYR:HA	1:D:471:LEU:HD12	1.62	0.80
1:E:378:VAL:HG21	1:E:390:ARG:HB2	1.64	0.80
1:F:342:HIS:HD2	1:F:344:LYS:H	1.26	0.80
1:A:480:ALA:HB2	1:E:174:MET:CE	2.11	0.80
1:C:141:TYR:O	1:C:144:VAL:HG12	1.83	0.79
1:F:258:ILE:HG21	1:F:273:LEU:HD13	1.62	0.79
1:A:378:VAL:HG21	1:A:390:ARG:HB2	1.63	0.79
1:F:2:VAL:CG2	1:F:45:GLU:HG3	2.12	0.79
1:A:11:ARG:H	1:A:14:GLN:NE2	1.81	0.78
1:A:139:GLY:HA2	1:E:241:SER:HB3	1.65	0.78
1:B:458:GLY:HA2	1:B:464:MET:HE1	1.65	0.78
1:A:116:LEU:HD11	1:A:123:LEU:HD22	1.66	0.78
1:E:11:ARG:H	1:E:14:GLN:NE2	1.80	0.78
1:A:208:ARG:HD3	1:A:474:LYS:CG	2.14	0.78
1:A:473:ALA:HB3	1:A:476:THR:HG21	1.63	0.78
1:C:330:SER:O	1:C:333:VAL:HG12	1.84	0.78
1:A:248:LYS:O	1:A:251:VAL:HG22	1.84	0.78
1:D:330:SER:O	1:D:333:VAL:HG12	1.83	0.78
1:E:169:THR:HG22	1:E:172:LYS:H	1.46	0.78
1:B:241:SER:CB	1:F:139:GLY:HA2	2.13	0.78
1:F:141:TYR:O	1:F:144:VAL:HG12	1.82	0.77
1:E:65:VAL:HG13	1:E:106:VAL:HG12	1.65	0.77
1:E:313:THR:HG22	1:E:316:SER:H	1.49	0.77
1:D:391:PHE:HB3	1:D:425:ALA:HB2	1.67	0.77
1:E:31:PRO:HD2	1:E:34:LEU:HD12	1.67	0.77
1:E:258:ILE:HG21	1:E:273:LEU:HD13	1.65	0.77
1:B:342:HIS:HD2	1:B:344:LYS:H	1.33	0.77
1:F:190:GLU:OE1	1:F:459:ARG:HD2	1.85	0.77
1:F:208:ARG:HD3	1:F:474:LYS:HD2	1.67	0.77
1:B:8:ILE:CD1	1:B:75:LEU:HD13	2.13	0.76
1:A:31:PRO:HD2	1:A:34:LEU:HD12	1.67	0.76
1:A:406:ARG:NH1	1:A:406:ARG:HB3	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:GLN:O	1:C:260:GLU:HG3	1.85	0.76
1:E:477:ARG:HB3	1:E:477:ARG:HH11	1.48	0.76
1:F:17:ILE:HG12	1:F:186:GLU:HG2	1.67	0.76
1:C:11:ARG:HG2	1:C:198:TYR:CD1	2.21	0.76
1:D:258:ILE:HG21	1:D:273:LEU:HD13	1.67	0.76
1:C:139:GLY:HA2	1:D:241:SER:HB2	1.66	0.76
1:F:330:SER:O	1:F:333:VAL:HG12	1.85	0.76
1:B:210:ASP:HA	1:B:474:LYS:HE3	1.68	0.75
1:F:11:ARG:HG2	1:F:198:TYR:CD1	2.22	0.75
1:B:139:GLY:HA2	1:F:241:SER:HB2	1.68	0.75
1:B:211:LEU:H	1:B:474:LYS:CE	1.99	0.75
1:B:169:THR:HG22	1:B:172:LYS:H	1.52	0.75
1:D:17:ILE:HG12	1:D:186:GLU:HG2	1.65	0.75
1:B:139:GLY:HA2	1:F:241:SER:CB	2.16	0.75
1:D:169:THR:HG22	1:D:172:LYS:H	1.52	0.75
1:A:256:GLN:O	1:A:260:GLU:HG3	1.86	0.75
1:F:291:THR:HG22	1:F:292:GLN:HG3	1.68	0.75
1:C:11:ARG:H	1:C:14:GLN:NE2	1.85	0.75
1:E:11:ARG:HG2	1:E:198:TYR:CD1	2.20	0.75
1:B:330:SER:O	1:B:333:VAL:HG12	1.86	0.74
1:C:17:ILE:HG12	1:C:186:GLU:HG2	1.67	0.74
1:E:248:LYS:O	1:E:251:VAL:HG22	1.85	0.74
1:A:458:GLY:HA2	1:A:464:MET:HE1	1.67	0.74
1:E:84:VAL:HG11	1:E:98:ALA:HB1	1.69	0.74
1:B:480:ALA:N	1:F:174:MET:HE3	2.03	0.74
1:D:248:LYS:O	1:D:251:VAL:HG22	1.87	0.74
1:F:473:ALA:HB3	1:F:476:THR:HG21	1.70	0.74
1:B:476:THR:HG22	1:B:477:ARG:H	1.52	0.73
1:B:258:ILE:HG21	1:B:273:LEU:HD13	1.68	0.73
1:C:84:VAL:HG11	1:C:98:ALA:HB1	1.70	0.73
1:E:330:SER:O	1:E:333:VAL:HG12	1.87	0.73
1:E:472:MET:CE	1:E:479:GLU:HA	2.18	0.73
1:E:208:ARG:NH1	1:E:474:LYS:HZ2	1.87	0.73
1:A:62:LYS:HG3	1:A:63:PRO:CD	2.19	0.73
1:A:174:MET:CE	1:E:480:ALA:HB2	2.16	0.73
1:D:123:LEU:H	1:D:123:LEU:CD2	2.02	0.73
1:E:17:ILE:HG12	1:E:186:GLU:HG2	1.71	0.73
1:D:1:MET:HE2	1:D:4:ARG:HA	1.71	0.72
1:B:190:GLU:OE1	1:B:459:ARG:HD2	1.89	0.72
1:B:256:GLN:O	1:B:260:GLU:HG3	1.89	0.72
1:A:391:PHE:HB3	1:A:425:ALA:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:HG11	1:A:98:ALA:HB1	1.71	0.72
1:F:211:LEU:N	1:F:474:LYS:HE2	1.99	0.72
1:D:11:ARG:H	1:D:14:GLN:HE21	1.34	0.72
1:B:208:ARG:HD3	1:B:474:LYS:HD3	1.72	0.72
1:A:8:ILE:HG13	1:A:10:PRO:HD3	1.72	0.72
1:D:31:PRO:HD2	1:D:34:LEU:HD12	1.72	0.72
1:D:342:HIS:HD2	1:D:344:LYS:H	1.37	0.71
1:A:123:LEU:H	1:A:123:LEU:CD2	2.04	0.71
1:B:17:ILE:HG12	1:B:186:GLU:HG2	1.72	0.71
1:C:313:THR:HG22	1:C:316:SER:H	1.54	0.71
1:A:17:ILE:HG12	1:A:186:GLU:HG2	1.72	0.71
1:A:190:GLU:OE1	1:A:459:ARG:HD2	1.90	0.71
1:B:248:LYS:O	1:B:251:VAL:HG22	1.90	0.71
1:D:84:VAL:HG11	1:D:98:ALA:HB1	1.71	0.71
1:E:458:GLY:HA2	1:E:464:MET:HE1	1.70	0.71
1:F:8:ILE:HG13	1:F:10:PRO:HD3	1.72	0.71
1:A:105:ILE:HD12	1:A:106:VAL:N	2.05	0.71
1:C:241:SER:CB	1:D:139:GLY:HA2	2.19	0.71
1:B:11:ARG:H	1:B:14:GLN:NE2	1.88	0.71
1:F:256:GLN:O	1:F:260:GLU:HG3	1.91	0.71
1:C:248:LYS:O	1:C:251:VAL:HG22	1.91	0.71
1:B:31:PRO:HD2	1:B:34:LEU:HD12	1.72	0.71
1:C:11:ARG:H	1:C:14:GLN:HE21	1.38	0.71
1:D:256:GLN:O	1:D:260:GLU:HG3	1.89	0.71
1:E:261:GLU:O	1:E:266:ASN:HB2	1.91	0.71
1:A:9:GLN:HB3	1:B:11:ARG:NH1	2.05	0.71
1:B:211:LEU:N	1:B:474:LYS:HE3	2.05	0.71
1:D:112:ILE:O	1:D:116:LEU:HB2	1.90	0.70
1:C:473:ALA:HB3	1:C:476:THR:CG2	2.22	0.70
1:F:406:ARG:HA	1:F:406:ARG:HH11	1.55	0.70
1:C:108:THR:OG1	1:C:111:THR:HG22	1.91	0.70
1:B:11:ARG:HG2	1:B:198:TYR:CD1	2.26	0.70
1:E:256:GLN:O	1:E:260:GLU:HG3	1.92	0.70
1:F:342:HIS:CD2	1:F:344:LYS:H	2.08	0.70
1:D:11:ARG:HG2	1:D:198:TYR:CD1	2.27	0.69
1:F:84:VAL:HG11	1:F:98:ALA:HB1	1.73	0.69
1:B:108:THR:OG1	1:B:111:THR:HG22	1.92	0.69
1:C:11:ARG:NH1	1:F:9:GLN:HB3	2.07	0.69
1:E:208:ARG:NE	1:E:474:LYS:HG2	2.08	0.69
1:A:11:ARG:H	1:A:14:GLN:HE21	1.38	0.69
1:D:1:MET:HE1	1:D:6:ASP:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:THR:OG1	1:F:111:THR:HG22	1.92	0.69
1:C:486:ARG:CZ	1:C:486:ARG:HA	2.21	0.69
1:D:22:LYS:HG2	1:D:46:TYR:CE2	2.28	0.69
1:D:261:GLU:O	1:D:266:ASN:HB2	1.92	0.69
1:E:108:THR:OG1	1:E:111:THR:HG22	1.93	0.69
1:B:84:VAL:HG11	1:B:98:ALA:HB1	1.74	0.68
1:C:112:ILE:O	1:C:116:LEU:HB2	1.94	0.68
1:A:108:THR:OG1	1:A:111:THR:HG22	1.93	0.68
1:B:219:ARG:O	1:B:223:ARG:HG3	1.93	0.68
1:E:407:GLU:OE1	1:E:407:GLU:N	2.26	0.68
1:F:11:ARG:HG2	1:F:198:TYR:CE1	2.28	0.68
1:D:262:MET:HE1	1:D:270:ARG:HG3	1.76	0.68
1:D:108:THR:OG1	1:D:111:THR:HG22	1.94	0.68
1:E:212:PRO:HD2	1:E:343:PRO:HG3	1.76	0.68
1:E:116:LEU:HD11	1:E:123:LEU:CD2	2.22	0.67
1:E:11:ARG:H	1:E:14:GLN:HE21	1.40	0.67
1:E:291:THR:HG22	1:E:292:GLN:HG3	1.76	0.67
1:F:473:ALA:HB3	1:F:476:THR:CG2	2.24	0.67
1:C:9:GLN:HB3	1:F:11:ARG:NH1	2.08	0.67
1:C:62:LYS:HE3	1:C:87:THR:OG1	1.95	0.67
1:C:291:THR:HG22	1:C:292:GLN:HG3	1.77	0.67
1:C:483:TRP:C	1:C:485:SER:H	2.02	0.67
1:A:62:LYS:HG3	1:A:63:PRO:HD3	1.76	0.67
1:B:112:ILE:O	1:B:116:LEU:HB2	1.94	0.67
1:C:11:ARG:HG2	1:C:198:TYR:CE1	2.28	0.67
1:A:313:THR:HG22	1:A:316:SER:H	1.59	0.67
1:D:320:PHE:O	1:D:326:LYS:HE2	1.95	0.67
1:F:211:LEU:H	1:F:474:LYS:CE	2.02	0.67
1:C:105:ILE:HD12	1:C:106:VAL:N	2.10	0.66
1:C:461:GLY:HA3	1:F:10:PRO:HG2	1.77	0.66
1:F:262:MET:HE1	1:F:270:ARG:HG3	1.77	0.66
1:A:174:MET:HE3	1:E:480:ALA:CB	2.24	0.66
1:A:480:ALA:CB	1:E:174:MET:HE3	2.23	0.66
1:C:473:ALA:HB3	1:C:476:THR:HG21	1.76	0.66
1:E:262:MET:HE1	1:E:270:ARG:HG3	1.76	0.66
1:A:262:MET:HE1	1:A:270:ARG:HG3	1.78	0.66
1:B:62:LYS:N	1:B:63:PRO:HD2	2.11	0.66
1:E:290:GLU:O	1:E:342:HIS:HE1	1.78	0.66
1:A:9:GLN:HB3	1:B:11:ARG:HH11	1.59	0.66
1:E:4:ARG:HB3	1:E:7:LEU:HG	1.77	0.66
1:E:112:ILE:O	1:E:116:LEU:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:SER:HB3	1:E:139:GLY:HA2	1.75	0.66
1:B:8:ILE:HD11	1:B:75:LEU:CD1	2.24	0.66
1:A:11:ARG:HG2	1:A:198:TYR:CD1	2.31	0.66
1:A:261:GLU:O	1:A:266:ASN:HB2	1.95	0.66
1:B:261:GLU:O	1:B:266:ASN:HB2	1.96	0.66
1:A:291:THR:HG22	1:A:292:GLN:HG3	1.78	0.66
1:C:219:ARG:O	1:C:223:ARG:HG3	1.94	0.66
1:C:25:ASN:ND2	1:C:159:VAL:H	1.93	0.66
1:E:11:ARG:HG2	1:E:198:TYR:CE1	2.30	0.65
1:A:112:ILE:O	1:A:116:LEU:HB2	1.95	0.65
1:C:485:SER:C	1:C:487:GLN:H	2.03	0.65
1:A:258:ILE:O	1:A:262:MET:HG3	1.97	0.65
1:B:185:ILE:HG21	1:B:187:TYR:CE1	2.31	0.65
1:C:391:PHE:HE1	1:C:412:LEU:HD13	1.61	0.65
1:F:112:ILE:O	1:F:116:LEU:HB2	1.97	0.65
1:A:36:LYS:HB2	2:A:495:PO4:O2	1.97	0.65
1:C:473:ALA:O	1:C:476:THR:HG22	1.97	0.65
1:E:342:HIS:CD2	1:E:344:LYS:H	2.10	0.65
1:F:47:ARG:HD3	1:F:158:LEU:HD12	1.79	0.65
1:A:486:ARG:NH2	1:E:166:PRO:HD2	2.10	0.65
1:D:258:ILE:O	1:D:262:MET:HG3	1.97	0.65
1:F:281:LYS:HD3	1:F:304:LEU:HD11	1.78	0.65
1:C:29:VAL:HB	1:C:187:TYR:HD2	1.61	0.65
1:C:281:LYS:HD3	1:C:304:LEU:HD11	1.78	0.65
1:E:105:ILE:HD12	1:E:106:VAL:N	2.11	0.65
1:A:342:HIS:HD2	1:A:344:LYS:H	1.43	0.65
1:B:47:ARG:HD3	1:B:158:LEU:HD12	1.77	0.65
1:C:31:PRO:HD2	1:C:34:LEU:HD12	1.79	0.65
1:B:258:ILE:O	1:B:262:MET:HG3	1.97	0.64
1:C:262:MET:HE1	1:C:270:ARG:HG3	1.79	0.64
1:A:173:ILE:HD12	1:E:484:SER:HB3	1.79	0.64
1:C:476:THR:HG23	1:C:478:ASP:N	2.08	0.64
1:D:105:ILE:HD12	1:D:106:VAL:N	2.12	0.64
1:D:116:LEU:HD11	1:D:123:LEU:CD2	2.28	0.64
1:D:219:ARG:O	1:D:223:ARG:HG3	1.98	0.64
1:C:441:VAL:HG22	1:C:468:VAL:HB	1.79	0.64
1:F:149:GLU:CD	1:F:152:ARG:HH12	2.06	0.64
1:A:258:ILE:HG21	1:A:273:LEU:HD13	1.79	0.64
1:B:142:ALA:O	1:B:146:ILE:HG13	1.96	0.64
1:C:22:LYS:HG2	1:C:46:TYR:CE2	2.33	0.64
1:F:13:TYR:CE1	1:F:14:GLN:HG3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLY:N	1:A:428:VAL:HG11	2.12	0.64
1:D:325:MET:O	1:D:329:ILE:HG13	1.98	0.64
1:F:5:ARG:HG2	1:F:5:ARG:HH11	1.63	0.64
1:B:291:THR:HG22	1:B:292:GLN:HG3	1.78	0.64
1:B:262:MET:HE1	1:B:270:ARG:HG3	1.79	0.64
1:D:355:GLN:HG3	1:D:440:LEU:HD22	1.80	0.64
1:E:208:ARG:NH1	1:E:474:LYS:NZ	2.45	0.64
1:D:62:LYS:N	1:D:63:PRO:HD2	2.14	0.63
1:E:258:ILE:O	1:E:262:MET:HG3	1.99	0.63
1:E:441:VAL:HG22	1:E:468:VAL:HB	1.79	0.63
1:A:320:PHE:O	1:A:326:LYS:HE2	1.99	0.63
1:B:123:LEU:H	1:B:123:LEU:CD2	2.07	0.63
1:B:282:LEU:O	1:B:286:ILE:HG12	1.99	0.63
1:C:342:HIS:HD2	1:C:344:LYS:H	1.45	0.63
1:E:208:ARG:HH12	1:E:474:LYS:HZ2	1.45	0.63
1:E:363:LYS:HD3	1:E:437:GLU:O	1.98	0.63
1:F:313:THR:HG22	1:F:316:SER:H	1.62	0.63
1:A:212:PRO:HD2	1:A:343:PRO:HG3	1.80	0.63
1:B:54:LYS:HB3	1:B:126:VAL:HA	1.81	0.63
1:B:342:HIS:CD2	1:B:344:LYS:H	2.17	0.63
1:C:14:GLN:HE22	1:F:9:GLN:HE22	1.46	0.63
1:A:241:SER:CB	1:E:139:GLY:HA2	2.28	0.63
1:B:1:MET:HE1	1:B:6:ASP:CG	2.24	0.63
1:D:291:THR:HG22	1:D:292:GLN:HG3	1.78	0.63
1:F:282:LEU:O	1:F:286:ILE:HG12	1.98	0.63
1:D:476:THR:HG23	1:D:478:ASP:N	2.13	0.63
1:E:485:SER:C	1:E:487:GLN:H	2.06	0.63
1:F:290:GLU:O	1:F:342:HIS:HE1	1.81	0.63
1:C:9:GLN:HB3	1:F:11:ARG:HH11	1.63	0.63
1:C:32:THR:HB	1:C:456:ARG:NH1	2.14	0.63
1:A:61:THR:O	1:A:65:VAL:HG23	1.99	0.62
1:B:477:ARG:HG2	1:B:477:ARG:HH11	1.64	0.62
1:B:174:MET:HE1	1:F:479:GLU:HG2	1.81	0.62
1:D:13:TYR:CE1	1:D:14:GLN:HG3	2.34	0.62
1:E:212:PRO:HD2	1:E:343:PRO:CG	2.29	0.62
1:B:290:GLU:O	1:B:342:HIS:HE1	1.82	0.62
1:C:116:LEU:HD11	1:C:123:LEU:CD2	2.29	0.62
1:E:281:LYS:HD3	1:E:304:LEU:HD11	1.80	0.62
1:E:282:LEU:O	1:E:286:ILE:HG12	1.99	0.62
1:B:174:MET:HE3	1:F:480:ALA:N	2.13	0.62
1:C:142:ALA:O	1:C:146:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:THR:HB	1:E:172:LYS:HB2	1.82	0.62
1:B:105:ILE:HD12	1:B:106:VAL:N	2.14	0.62
1:F:261:GLU:O	1:F:266:ASN:HB2	2.00	0.62
1:A:133:GLU:O	1:A:136:ARG:HG2	1.99	0.62
1:C:36:LYS:HE3	2:C:495:PO4:O1	1.98	0.62
1:B:441:VAL:HG22	1:B:468:VAL:HB	1.80	0.62
1:C:8:ILE:HG12	1:C:10:PRO:HD3	1.81	0.62
1:F:62:LYS:N	1:F:63:PRO:HD2	2.15	0.62
1:F:123:LEU:H	1:F:123:LEU:CD2	2.09	0.62
1:C:476:THR:OG1	1:C:477:ARG:N	2.32	0.62
1:B:116:LEU:HD11	1:B:123:LEU:CD2	2.29	0.62
1:B:169:THR:HB	1:B:172:LYS:HB2	1.81	0.62
1:D:212:PRO:HD2	1:D:343:PRO:HG2	1.82	0.62
1:A:116:LEU:HD11	1:A:123:LEU:CD2	2.28	0.62
1:C:123:LEU:H	1:C:123:LEU:CD2	2.11	0.62
1:C:406:ARG:HD3	1:C:406:ARG:N	2.12	0.62
1:C:325:MET:O	1:C:329:ILE:HG13	2.00	0.61
1:A:219:ARG:O	1:A:223:ARG:HG3	2.00	0.61
1:B:453:SER:O	1:B:457:ARG:HG2	1.99	0.61
1:E:482:TYR:O	1:E:486:ARG:HB2	2.01	0.61
1:D:11:ARG:NH2	1:D:459:ARG:O	2.33	0.61
1:B:11:ARG:HG2	1:B:198:TYR:CE1	2.36	0.61
1:C:139:GLY:CA	1:D:241:SER:HB3	2.29	0.61
1:C:62:LYS:HE3	1:C:87:THR:HG1	1.63	0.61
1:E:123:LEU:H	1:E:123:LEU:CD2	2.09	0.61
1:F:31:PRO:HD2	1:F:34:LEU:HD12	1.81	0.61
1:F:258:ILE:O	1:F:262:MET:HG3	2.00	0.61
1:C:290:GLU:O	1:C:342:HIS:HE1	1.84	0.61
1:F:248:LYS:O	1:F:251:VAL:HG22	1.99	0.61
1:A:355:GLN:NE2	1:A:358:ARG:HH22	1.99	0.61
1:C:11:ARG:HH11	1:F:9:GLN:HB3	1.66	0.61
1:C:13:TYR:CE1	1:C:14:GLN:HG3	2.35	0.61
1:F:177:ILE:HG23	1:F:182:ILE:HB	1.83	0.61
1:E:27:LEU:HD13	1:E:182:ILE:HG13	1.81	0.61
1:F:320:PHE:O	1:F:326:LYS:HE2	2.00	0.61
1:F:483:TRP:C	1:F:485:SER:H	2.09	0.61
1:F:105:ILE:HD12	1:F:106:VAL:N	2.15	0.61
1:C:62:LYS:N	1:C:63:PRO:HD2	2.16	0.60
1:C:323:LYS:O	1:C:326:LYS:HB2	2.01	0.60
1:D:461:GLY:HA3	1:E:10:PRO:HG2	1.83	0.60
1:F:477:ARG:HG2	1:F:477:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ALA:HA	1:B:239:LEU:HD23	1.84	0.60
1:E:208:ARG:CZ	1:E:474:LYS:HG2	2.31	0.60
1:E:222:LEU:HB3	1:E:286:ILE:HD13	1.82	0.60
1:E:320:PHE:O	1:E:326:LYS:HE2	2.01	0.60
1:F:116:LEU:HD11	1:F:123:LEU:CD2	2.31	0.60
1:C:480:ALA:N	1:D:174:MET:HE3	2.16	0.60
1:A:234:ALA:HA	1:A:239:LEU:HD23	1.83	0.60
1:B:392:VAL:HG22	1:B:393:GLY:H	1.66	0.60
1:D:169:THR:HB	1:D:172:LYS:HB2	1.84	0.60
1:E:392:VAL:HG22	1:E:392:VAL:O	2.02	0.60
1:A:483:TRP:O	1:A:485:SER:N	2.35	0.60
1:C:2:VAL:HB	1:C:45:GLU:HG3	1.84	0.60
1:D:345:MET:HE2	1:D:380:GLU:HG2	1.83	0.60
1:F:169:THR:HB	1:F:172:LYS:HB2	1.84	0.60
1:F:391:PHE:HE2	1:F:408:GLN:NE2	2.00	0.60
1:E:8:ILE:HD11	1:E:75:LEU:HD13	1.83	0.60
1:E:47:ARG:HD3	1:E:158:LEU:HD12	1.82	0.60
1:E:169:THR:HG23	1:E:171:GLU:OE2	2.01	0.60
1:A:212:PRO:HD2	1:A:343:PRO:CG	2.31	0.60
1:A:453:SER:O	1:A:457:ARG:HG2	2.01	0.60
1:C:320:PHE:O	1:C:326:LYS:HE2	2.01	0.60
1:C:391:PHE:HD2	1:C:391:PHE:C	2.10	0.60
1:E:222:LEU:HB3	1:E:286:ILE:CD1	2.31	0.60
1:D:281:LYS:HD3	1:D:304:LEU:HD11	1.84	0.59
1:E:456:ARG:HH11	1:E:456:ARG:HG2	1.67	0.59
1:A:212:PRO:CD	1:A:343:PRO:HG3	2.31	0.59
1:D:11:ARG:HG2	1:D:198:TYR:CE1	2.38	0.59
1:D:282:LEU:O	1:D:286:ILE:HG12	2.03	0.59
1:C:196:ARG:HB2	1:C:197:PRO:HD3	1.82	0.59
1:C:355:GLN:HG3	1:C:440:LEU:HD22	1.84	0.59
1:B:222:LEU:HB3	1:B:286:ILE:HD13	1.84	0.59
1:D:177:ILE:HG23	1:D:182:ILE:HB	1.84	0.59
1:C:47:ARG:HD3	1:C:158:LEU:HD12	1.83	0.59
1:D:426:THR:CG2	1:D:428:VAL:HG12	2.30	0.59
1:F:208:ARG:HD3	1:F:474:LYS:CD	2.31	0.59
1:C:27:LEU:HD13	1:C:182:ILE:HG13	1.85	0.59
1:C:458:GLY:CA	1:C:464:MET:HE1	2.33	0.59
1:D:135:HIS:HE1	3:D:501:HOH:O	1.84	0.59
1:A:391:PHE:CE2	1:A:429:GLY:HA2	2.38	0.58
1:E:13:TYR:CE1	1:E:14:GLN:HG3	2.38	0.58
1:A:208:ARG:HD3	1:A:474:LYS:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:PHE:CE1	1:B:412:LEU:HD13	2.38	0.58
1:D:374:ALA:O	1:D:378:VAL:HG23	2.03	0.58
1:D:456:ARG:HG2	1:D:456:ARG:HH11	1.67	0.58
1:E:22:LYS:HD2	1:E:46:TYR:CD1	2.37	0.58
1:A:456:ARG:HG2	1:A:456:ARG:HH11	1.69	0.58
1:B:196:ARG:HB2	1:B:197:PRO:HD3	1.85	0.58
1:F:260:GLU:O	1:F:264:LYS:HG3	2.03	0.58
1:A:208:ARG:HD3	1:A:474:LYS:HG3	1.85	0.58
1:E:234:ALA:HA	1:E:239:LEU:HD23	1.85	0.58
1:C:54:LYS:HB3	1:C:126:VAL:HA	1.85	0.58
1:C:207:VAL:CG2	1:C:471:LEU:HD23	2.33	0.58
1:D:47:ARG:HD3	1:D:158:LEU:HD12	1.85	0.58
1:D:142:ALA:O	1:D:146:ILE:HG13	2.03	0.58
1:D:453:SER:O	1:D:457:ARG:HG2	2.02	0.58
1:F:355:GLN:HG3	1:F:440:LEU:HD22	1.85	0.58
1:C:261:GLU:O	1:C:266:ASN:HB2	2.03	0.58
1:D:234:ALA:HA	1:D:239:LEU:HD23	1.85	0.58
1:D:473:ALA:HB3	1:D:476:THR:HG21	1.86	0.58
1:E:62:LYS:N	1:E:63:PRO:HD2	2.18	0.58
1:A:50:LYS:HD3	1:A:51:TYR:CZ	2.39	0.58
1:B:355:GLN:HG3	1:B:440:LEU:HD22	1.86	0.58
1:C:391:PHE:CE1	1:C:412:LEU:HD13	2.38	0.58
1:A:392:VAL:HG22	1:A:393:GLY:N	2.18	0.58
1:F:325:MET:O	1:F:329:ILE:HG13	2.04	0.58
1:A:169:THR:HG23	1:A:171:GLU:OE2	2.03	0.58
1:C:190:GLU:OE1	1:C:459:ARG:HD2	2.04	0.58
1:D:32:THR:HB	1:D:456:ARG:NH1	2.19	0.58
1:D:290:GLU:O	1:D:342:HIS:HE1	1.87	0.58
1:D:34:LEU:HG	1:D:459:ARG:HG2	1.85	0.57
1:D:54:LYS:HB3	1:D:126:VAL:HA	1.86	0.57
1:B:287:GLU:O	1:B:291:THR:HB	2.04	0.57
1:A:1:MET:HE2	1:B:462:ARG:NE	2.18	0.57
1:F:391:PHE:HB3	1:F:425:ALA:HB2	1.86	0.57
1:F:458:GLY:CA	1:F:464:MET:HE1	2.32	0.57
1:A:62:LYS:N	1:A:63:PRO:HD2	2.20	0.57
1:C:234:ALA:HA	1:C:239:LEU:HD23	1.85	0.57
1:C:391:PHE:HB2	1:C:423:LEU:HD11	1.86	0.57
1:D:149:GLU:CD	1:D:152:ARG:HH12	2.13	0.57
1:E:219:ARG:O	1:E:223:ARG:HG3	2.05	0.57
1:A:142:ALA:O	1:A:146:ILE:HG13	2.05	0.57
1:A:355:GLN:HG3	1:A:440:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:LEU:HG	1:D:105:ILE:HD13	1.86	0.57
1:D:196:ARG:HB2	1:D:197:PRO:HD3	1.86	0.57
1:F:22:LYS:HG2	1:F:46:TYR:CE2	2.39	0.57
1:B:8:ILE:HB	1:B:10:PRO:HD3	1.85	0.57
1:D:390:ARG:NH1	1:D:390:ARG:HG2	2.19	0.57
1:D:452:ARG:HD2	1:D:456:ARG:NH2	2.19	0.57
1:E:325:MET:O	1:E:329:ILE:HG13	2.05	0.57
1:F:234:ALA:HA	1:F:239:LEU:HD23	1.86	0.57
1:B:426:THR:CG2	1:B:428:VAL:HG12	2.31	0.57
1:A:472:MET:HE1	1:A:482:TYR:HB2	1.86	0.57
1:C:86:LEU:HB2	1:C:107:ALA:HB2	1.87	0.57
1:A:177:ILE:HG23	1:A:182:ILE:HB	1.85	0.56
1:A:208:ARG:NE	1:A:474:LYS:HG2	2.19	0.56
1:E:355:GLN:HG3	1:E:440:LEU:HD22	1.88	0.56
1:B:22:LYS:HG2	1:B:46:TYR:CE2	2.40	0.56
1:B:456:ARG:HG2	1:B:456:ARG:HH11	1.70	0.56
1:C:282:LEU:O	1:C:286:ILE:HG12	2.06	0.56
1:C:291:THR:CG2	1:C:292:GLN:HE21	2.18	0.56
1:D:135:HIS:H	1:D:135:HIS:CD2	2.23	0.56
1:F:5:ARG:HG2	1:F:5:ARG:NH1	2.21	0.56
1:F:355:GLN:NE2	1:F:358:ARG:HH22	2.03	0.56
1:B:13:TYR:CE1	1:B:14:GLN:HG3	2.41	0.56
1:F:54:LYS:HB3	1:F:126:VAL:HA	1.86	0.56
1:A:282:LEU:O	1:A:286:ILE:HG12	2.05	0.56
1:B:11:ARG:NH2	1:B:459:ARG:O	2.38	0.56
1:C:169:THR:HB	1:C:172:LYS:HB2	1.88	0.56
1:C:258:ILE:O	1:C:262:MET:HG3	2.06	0.56
1:C:456:ARG:HG2	1:C:456:ARG:HH11	1.69	0.56
1:D:25:ASN:ND2	1:D:159:VAL:H	2.02	0.56
1:D:462:ARG:HG2	1:E:1:MET:HE1	1.87	0.56
1:F:407:GLU:O	1:F:411:ILE:HG22	2.05	0.56
1:A:169:THR:HB	1:A:172:LYS:HB2	1.87	0.56
1:C:185:ILE:HB	1:D:483:TRP:CZ3	2.41	0.56
1:D:476:THR:CG2	1:D:478:ASP:HB2	2.36	0.56
1:F:391:PHE:HB2	1:F:423:LEU:HD11	1.87	0.56
1:C:481:TYR:O	1:C:485:SER:HB3	2.06	0.56
1:F:219:ARG:O	1:F:223:ARG:HG3	2.06	0.56
1:A:458:GLY:CA	1:A:464:MET:HE1	2.34	0.56
1:A:473:ALA:HB3	1:A:476:THR:CG2	2.33	0.56
1:C:22:LYS:HD2	1:C:46:TYR:CD1	2.41	0.56
1:C:86:LEU:HG	1:C:105:ILE:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:THR:CG2	1:C:428:VAL:HG12	2.28	0.56
1:B:86:LEU:HG	1:B:105:ILE:HD13	1.87	0.56
1:D:86:LEU:HB2	1:D:107:ALA:HB2	1.88	0.56
1:B:25:ASN:ND2	1:B:159:VAL:H	2.04	0.56
1:C:241:SER:HB2	1:D:139:GLY:CA	2.27	0.56
1:D:231:LYS:O	1:D:235:GLU:HG3	2.06	0.56
1:F:86:LEU:HG	1:F:105:ILE:HD13	1.87	0.56
1:A:208:ARG:CD	1:A:474:LYS:HG2	2.37	0.55
1:A:480:ALA:HB2	1:E:174:MET:HG2	1.87	0.55
1:A:391:PHE:HB2	1:A:423:LEU:HD11	1.88	0.55
1:A:287:GLU:O	1:A:291:THR:HB	2.06	0.55
1:B:260:GLU:O	1:B:264:LYS:HG3	2.05	0.55
1:A:105:ILE:HD12	1:A:105:ILE:C	2.32	0.55
1:C:391:PHE:HB3	1:C:425:ALA:HB2	1.88	0.55
1:D:407:GLU:O	1:D:411:ILE:HG22	2.06	0.55
1:E:407:GLU:O	1:E:411:ILE:HG22	2.07	0.55
1:F:196:ARG:HB2	1:F:197:PRO:HD3	1.88	0.55
1:A:222:LEU:HB3	1:A:286:ILE:HD13	1.87	0.55
1:A:366:VAL:HG22	1:A:442:VAL:HG13	1.88	0.55
1:B:27:LEU:HD13	1:B:182:ILE:HG13	1.88	0.55
1:B:61:THR:O	1:B:65:VAL:HG23	2.06	0.55
1:A:290:GLU:O	1:A:342:HIS:HE1	1.89	0.55
1:A:374:ALA:O	1:A:378:VAL:HG23	2.06	0.55
1:C:391:PHE:C	1:C:391:PHE:CD2	2.82	0.55
1:C:443:PHE:CD2	1:C:470:ILE:HD13	2.42	0.55
1:A:86:LEU:HG	1:A:105:ILE:HD13	1.89	0.55
1:C:222:LEU:HB3	1:C:286:ILE:HD13	1.89	0.55
1:E:392:VAL:HG13	1:E:408:GLN:HE21	1.71	0.55
1:A:47:ARG:HD3	1:A:158:LEU:HD12	1.88	0.55
1:A:174:MET:HE2	1:A:177:ILE:HD12	1.89	0.55
1:F:25:ASN:ND2	1:F:159:VAL:H	2.04	0.55
1:F:363:LYS:HD3	1:F:437:GLU:O	2.07	0.55
1:C:407:GLU:O	1:C:411:ILE:HG22	2.07	0.55
1:F:22:LYS:HD2	1:F:46:TYR:CD1	2.42	0.55
1:C:452:ARG:HD2	1:C:456:ARG:NH2	2.22	0.54
1:F:391:PHE:C	1:F:391:PHE:CD2	2.85	0.54
1:F:444:TYR:HA	1:F:471:LEU:HD12	1.87	0.54
1:A:11:ARG:HG2	1:A:198:TYR:CE1	2.42	0.54
1:A:54:LYS:HB3	1:A:126:VAL:HA	1.89	0.54
1:C:226:LEU:HD22	1:C:230:LEU:CD1	2.37	0.54
1:E:86:LEU:HB2	1:E:107:ALA:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:456:ARG:HG2	1:F:456:ARG:HH11	1.72	0.54
1:F:441:VAL:HG22	1:F:468:VAL:HB	1.89	0.54
1:D:204:PHE:HD2	1:D:468:VAL:HG21	1.72	0.54
1:D:390:ARG:HG2	1:D:390:ARG:HH11	1.71	0.54
1:B:32:THR:HA	2:B:495:PO4:O3	2.07	0.54
1:B:225:MET:HG2	1:B:324:ARG:HH21	1.72	0.54
1:E:86:LEU:HG	1:E:105:ILE:HD13	1.90	0.54
1:C:391:PHE:HE2	1:C:408:GLN:NE2	2.05	0.54
1:F:2:VAL:HG21	1:F:45:GLU:HG3	1.89	0.54
1:A:50:LYS:HD3	1:A:51:TYR:CE1	2.43	0.54
1:B:11:ARG:H	1:B:14:GLN:HE21	1.55	0.54
1:E:364:ILE:CG1	1:E:422:VAL:HG22	2.37	0.54
1:E:177:ILE:HG23	1:E:182:ILE:HB	1.90	0.54
1:F:426:THR:CG2	1:F:428:VAL:HG12	2.28	0.54
1:A:196:ARG:HB2	1:A:197:PRO:HD3	1.90	0.53
1:C:8:ILE:HG22	1:C:75:LEU:HD22	1.88	0.53
1:D:355:GLN:NE2	1:D:358:ARG:HH22	2.05	0.53
1:D:363:LYS:HD3	1:D:437:GLU:O	2.07	0.53
1:A:187:TYR:O	1:A:188:ARG:HD3	2.08	0.53
1:B:60:PRO:HG3	1:B:136:ARG:HD3	1.90	0.53
1:B:320:PHE:O	1:B:326:LYS:HE2	2.08	0.53
1:C:50:LYS:HD3	1:C:51:TYR:CZ	2.43	0.53
1:C:485:SER:C	1:C:487:GLN:N	2.66	0.53
1:E:36:LYS:N	2:E:495:PO4:O3	2.41	0.53
1:F:390:ARG:NH1	1:F:390:ARG:HG2	2.22	0.53
1:F:452:ARG:HD2	1:F:456:ARG:NH2	2.24	0.53
1:F:483:TRP:C	1:F:485:SER:N	2.65	0.53
1:E:458:GLY:CA	1:E:464:MET:HE1	2.39	0.53
1:B:86:LEU:HB2	1:B:107:ALA:HB2	1.90	0.53
1:C:276:HIS:CE1	1:C:280:LEU:HD22	2.44	0.53
1:D:276:HIS:CE1	1:D:280:LEU:HD22	2.44	0.53
1:F:204:PHE:HD2	1:F:468:VAL:HG21	1.74	0.53
1:D:113:GLU:HG3	1:D:145:PHE:CD2	2.43	0.53
1:D:253:ARG:NH1	1:D:257:ILE:HG12	2.23	0.53
1:D:441:VAL:HG22	1:D:468:VAL:HB	1.91	0.53
1:F:169:THR:HG22	1:F:172:LYS:N	2.12	0.53
1:A:407:GLU:O	1:A:411:ILE:HG22	2.09	0.53
1:D:34:LEU:CD2	1:D:459:ARG:HG2	2.39	0.53
1:D:123:LEU:HD23	1:D:123:LEU:N	2.07	0.53
1:F:2:VAL:HG22	1:F:45:GLU:OE2	2.09	0.53
1:B:50:LYS:HD3	1:B:51:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:ALA:CA	1:D:174:MET:HE3	2.39	0.53
1:A:86:LEU:HB2	1:A:107:ALA:HB2	1.90	0.53
1:A:325:MET:O	1:A:329:ILE:HG13	2.09	0.53
1:A:364:ILE:CG1	1:A:422:VAL:HG22	2.39	0.53
1:E:313:THR:CG2	1:E:316:SER:H	2.19	0.53
1:A:406:ARG:HH11	1:A:406:ARG:CB	2.22	0.52
1:B:204:PHE:HD2	1:B:468:VAL:HG21	1.74	0.52
1:B:364:ILE:CG1	1:B:422:VAL:HG22	2.39	0.52
1:C:149:GLU:CD	1:C:152:ARG:HH12	2.17	0.52
1:C:342:HIS:CD2	1:C:344:LYS:H	2.25	0.52
1:D:48:LEU:HD21	1:D:55:VAL:HG23	1.90	0.52
1:D:55:VAL:HG13	1:D:128:LEU:HD23	1.91	0.52
1:D:222:LEU:HB3	1:D:286:ILE:HD13	1.90	0.52
1:E:204:PHE:HD2	1:E:468:VAL:HG21	1.73	0.52
1:E:392:VAL:C	1:E:408:GLN:HE21	2.17	0.52
1:F:142:ALA:O	1:F:146:ILE:HG13	2.09	0.52
1:A:222:LEU:HB3	1:A:286:ILE:CD1	2.38	0.52
1:A:345:MET:HE2	1:A:380:GLU:HG2	1.91	0.52
1:C:437:GLU:O	1:C:437:GLU:HG2	2.09	0.52
1:D:204:PHE:CD2	1:D:468:VAL:HG21	2.43	0.52
1:F:453:SER:O	1:F:457:ARG:HG2	2.09	0.52
1:A:36:LYS:H	2:A:495:PO4:P	2.33	0.52
1:B:30:LEU:HD22	1:B:188:ARG:HB3	1.91	0.52
1:B:222:LEU:HB3	1:B:286:ILE:CD1	2.40	0.52
1:E:133:GLU:O	1:E:136:ARG:HG2	2.10	0.52
1:B:325:MET:O	1:B:329:ILE:HG13	2.10	0.52
1:B:391:PHE:C	1:B:391:PHE:CD2	2.87	0.52
1:D:1:MET:CE	1:D:5:ARG:N	2.72	0.52
1:A:476:THR:HG23	1:A:478:ASP:H	1.75	0.52
1:F:8:ILE:CG1	1:F:10:PRO:HD3	2.38	0.52
1:B:98:ALA:HA	1:B:101:ARG:NH1	2.24	0.52
1:C:453:SER:O	1:C:457:ARG:HG2	2.09	0.52
1:D:222:LEU:HB3	1:D:286:ILE:CD1	2.40	0.52
1:E:261:GLU:OE1	1:E:264:LYS:HD2	2.10	0.52
1:F:206:TRP:CG	1:F:482:TYR:HD2	2.27	0.52
1:A:149:GLU:CD	1:A:152:ARG:HH12	2.17	0.52
1:A:483:TRP:C	1:A:485:SER:N	2.66	0.52
1:C:260:GLU:O	1:C:264:LYS:HG3	2.09	0.52
1:D:477:ARG:HB3	1:D:477:ARG:HH11	1.71	0.52
1:A:208:ARG:CZ	1:A:474:LYS:HG2	2.39	0.52
1:B:8:ILE:HD11	1:B:75:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:GLU:HG3	1:C:145:PHE:CD2	2.45	0.52
1:E:258:ILE:CG2	1:E:273:LEU:HD13	2.39	0.52
1:F:222:LEU:HB3	1:F:286:ILE:HD13	1.91	0.52
1:C:10:PRO:HG2	1:F:461:GLY:HA3	1.91	0.52
1:C:36:LYS:N	2:C:495:PO4:O3	2.43	0.52
1:C:390:ARG:NH1	1:C:390:ARG:HG2	2.24	0.52
1:C:483:TRP:C	1:C:485:SER:N	2.64	0.52
1:F:391:PHE:HD2	1:F:392:VAL:N	2.08	0.52
1:B:476:THR:HG22	1:B:477:ARG:N	2.22	0.52
1:C:313:THR:CG2	1:C:316:SER:H	2.21	0.52
1:C:364:ILE:HB	1:C:440:LEU:HD23	1.92	0.52
1:E:192:SER:O	1:E:196:ARG:HG3	2.10	0.52
1:F:12:ILE:HG13	1:F:198:TYR:OH	2.10	0.52
1:F:113:GLU:HG3	1:F:145:PHE:CD2	2.45	0.52
1:B:149:GLU:CD	1:B:152:ARG:HH12	2.17	0.51
1:D:477:ARG:HB3	1:D:477:ARG:CZ	2.39	0.51
1:E:149:GLU:CD	1:E:152:ARG:HH12	2.17	0.51
1:F:86:LEU:HB2	1:F:107:ALA:HB2	1.90	0.51
1:A:173:ILE:CD1	1:E:484:SER:HB3	2.40	0.51
1:A:363:LYS:HD3	1:A:437:GLU:O	2.10	0.51
1:C:374:ALA:O	1:C:378:VAL:HG23	2.11	0.51
1:E:54:LYS:HB3	1:E:126:VAL:HA	1.92	0.51
1:E:196:ARG:HB2	1:E:197:PRO:HD3	1.92	0.51
1:A:31:PRO:HD2	1:A:34:LEU:CD1	2.40	0.51
1:A:392:VAL:HG22	1:A:393:GLY:H	1.74	0.51
1:C:258:ILE:CG2	1:C:273:LEU:HD13	2.36	0.51
1:F:204:PHE:CD2	1:F:468:VAL:HG21	2.45	0.51
1:F:206:TRP:CH2	1:F:485:SER:HB3	2.45	0.51
1:A:393:GLY:HA3	1:A:428:VAL:HG21	1.93	0.51
1:B:139:GLY:HA2	1:F:241:SER:HB3	1.92	0.51
1:C:83:ILE:HD13	1:C:104:VAL:HB	1.93	0.51
1:E:248:LYS:HG2	1:E:252:LEU:HD21	1.92	0.51
1:A:3:LEU:HD13	1:A:76:PHE:CZ	2.45	0.51
1:A:36:LYS:HE3	2:A:495:PO4:P	2.50	0.51
1:A:390:ARG:NH1	1:A:390:ARG:HG2	2.25	0.51
1:B:390:ARG:NH1	1:B:390:ARG:HG2	2.25	0.51
1:D:30:LEU:HD22	1:D:188:ARG:HB3	1.91	0.51
1:E:207:VAL:HG22	1:E:471:LEU:HD23	1.92	0.51
1:F:225:MET:HG2	1:F:324:ARG:HH21	1.75	0.51
1:F:390:ARG:HG2	1:F:390:ARG:HH11	1.75	0.51
1:B:135:HIS:CD2	1:B:135:HIS:H	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:CE	1:D:5:ARG:H	2.23	0.51
1:A:13:TYR:CE1	1:A:14:GLN:HG3	2.46	0.51
1:A:333:VAL:CG1	1:A:334:GLN:N	2.74	0.51
1:A:406:ARG:NH1	1:A:406:ARG:CB	2.72	0.51
1:A:472:MET:HB3	1:A:478:ASP:HB3	1.91	0.51
1:C:177:ILE:HG23	1:C:182:ILE:HB	1.93	0.51
1:D:225:MET:HG2	1:D:324:ARG:HH21	1.76	0.51
1:E:355:GLN:NE2	1:E:358:ARG:HH22	2.09	0.51
1:F:364:ILE:HB	1:F:440:LEU:HD23	1.91	0.51
1:F:366:VAL:HG22	1:F:442:VAL:HG13	1.93	0.51
1:B:391:PHE:HE1	1:B:412:LEU:HD13	1.76	0.51
1:C:486:ARG:HA	1:C:486:ARG:NH1	2.25	0.51
1:E:260:GLU:O	1:E:264:LYS:HG3	2.10	0.51
1:F:261:GLU:OE1	1:F:264:LYS:HD2	2.10	0.51
1:E:50:LYS:HD3	1:E:51:TYR:CZ	2.45	0.51
1:E:50:LYS:HD3	1:E:51:TYR:CE1	2.46	0.51
1:F:365:ILE:O	1:F:441:VAL:HA	2.10	0.51
1:B:177:ILE:HG23	1:B:182:ILE:HB	1.92	0.51
1:E:248:LYS:HG2	1:E:252:LEU:CD2	2.41	0.51
1:E:434:ASP:OD1	1:E:462:ARG:NH2	2.42	0.51
1:E:472:MET:HE1	1:E:482:TYR:HB2	1.93	0.51
1:A:365:ILE:O	1:A:441:VAL:HA	2.11	0.50
1:E:453:SER:O	1:E:457:ARG:HG2	2.11	0.50
1:F:248:LYS:HG2	1:F:252:LEU:CD2	2.40	0.50
1:A:75:LEU:HD11	1:B:7:LEU:HD22	1.93	0.50
1:C:169:THR:HG23	1:C:171:GLU:OE2	2.12	0.50
1:D:230:LEU:HD22	1:D:239:LEU:HD11	1.93	0.50
1:D:281:LYS:HG3	3:D:502:HOH:O	2.10	0.50
1:E:366:VAL:HG22	1:E:442:VAL:HG13	1.93	0.50
1:E:486:ARG:O	1:E:486:ARG:HD3	2.11	0.50
1:A:174:MET:HG2	1:E:480:ALA:HB2	1.92	0.50
1:A:248:LYS:HG2	1:A:252:LEU:HD21	1.92	0.50
1:C:11:ARG:NH2	1:C:459:ARG:O	2.45	0.50
1:C:230:LEU:HD22	1:C:239:LEU:HD11	1.93	0.50
1:E:22:LYS:HG2	1:E:46:TYR:CE2	2.45	0.50
1:F:2:VAL:HG22	1:F:45:GLU:HG3	1.93	0.50
1:F:364:ILE:HD11	1:F:366:VAL:HG23	1.94	0.50
1:A:394:GLN:HG2	1:A:405:GLN:N	2.26	0.50
1:A:441:VAL:HG22	1:A:468:VAL:HB	1.94	0.50
1:B:113:GLU:HG3	1:B:145:PHE:CD2	2.47	0.50
1:C:241:SER:CB	1:D:139:GLY:CA	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:ARG:HG2	1:C:390:ARG:HH11	1.77	0.50
1:A:122:SER:OG	1:A:124:GLU:CG	2.60	0.50
1:A:248:LYS:HG2	1:A:252:LEU:CD2	2.41	0.50
1:B:241:SER:HB3	1:F:139:GLY:HA2	1.93	0.50
1:B:268:ASP:C	1:B:270:ARG:H	2.19	0.50
1:D:323:LYS:O	1:D:326:LYS:HB2	2.10	0.50
1:E:485:SER:C	1:E:487:GLN:N	2.69	0.50
1:F:123:LEU:HD23	1:F:123:LEU:N	2.16	0.50
1:F:135:HIS:H	1:F:135:HIS:CD2	2.29	0.50
1:B:363:LYS:HD3	1:B:437:GLU:O	2.12	0.50
1:C:248:LYS:HG2	1:C:252:LEU:CD2	2.42	0.50
1:C:248:LYS:HG2	1:C:252:LEU:HD21	1.94	0.50
1:F:258:ILE:CG2	1:F:273:LEU:HD13	2.36	0.50
1:F:374:ALA:O	1:F:378:VAL:HG23	2.12	0.50
1:F:477:ARG:HG2	1:F:477:ARG:NH1	2.25	0.50
1:B:258:ILE:CG2	1:B:273:LEU:HD13	2.41	0.50
1:D:260:GLU:O	1:D:264:LYS:HG3	2.11	0.50
1:D:477:ARG:CZ	1:D:477:ARG:CB	2.90	0.50
1:F:268:ASP:C	1:F:270:ARG:H	2.19	0.50
1:C:174:MET:HE3	1:D:480:ALA:CA	2.42	0.50
1:E:472:MET:HE2	1:E:479:GLU:CA	2.31	0.50
1:C:204:PHE:HD2	1:C:468:VAL:HG21	1.76	0.49
1:C:364:ILE:CG1	1:C:422:VAL:HG22	2.41	0.49
1:E:294:LEU:HD12	1:E:340:LEU:O	2.11	0.49
1:F:124:GLU:HB3	1:F:153:GLN:O	2.11	0.49
1:F:364:ILE:CG1	1:F:422:VAL:HG22	2.41	0.49
1:A:323:LYS:O	1:A:326:LYS:HB2	2.11	0.49
1:A:406:ARG:HB3	1:A:406:ARG:CZ	2.42	0.49
1:D:11:ARG:HH11	1:E:9:GLN:HB3	1.77	0.49
1:F:222:LEU:HB3	1:F:286:ILE:CD1	2.41	0.49
1:A:472:MET:HE2	1:A:479:GLU:HA	1.94	0.49
1:B:452:ARG:HD2	1:B:456:ARG:NH2	2.27	0.49
1:C:98:ALA:HA	1:C:101:ARG:NH1	2.26	0.49
1:C:135:HIS:H	1:C:135:HIS:CD2	2.29	0.49
1:C:355:GLN:NE2	1:C:358:ARG:HH22	2.10	0.49
1:D:243:SER:C	1:D:245:ASP:H	2.20	0.49
1:A:207:VAL:HG22	1:A:471:LEU:HD23	1.94	0.49
1:B:407:GLU:O	1:B:411:ILE:HG22	2.11	0.49
1:E:364:ILE:HG13	1:E:422:VAL:HG22	1.95	0.49
1:F:345:MET:HE2	1:F:380:GLU:HG2	1.95	0.49
1:C:253:ARG:O	1:C:257:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:PHE:HD2	1:C:392:VAL:N	2.10	0.49
1:C:473:ALA:HB3	1:C:476:THR:HG22	1.93	0.49
1:D:1:MET:CE	1:D:6:ASP:H	2.23	0.49
1:D:212:PRO:HD2	1:D:343:PRO:CG	2.42	0.49
1:E:169:THR:HG22	1:E:171:GLU:N	2.26	0.49
1:B:354:GLU:OE1	1:B:358:ARG:NH1	2.46	0.49
1:C:8:ILE:CG2	1:C:75:LEU:HD22	2.42	0.49
1:A:109:PRO:HB2	1:A:142:ALA:HB3	1.94	0.49
1:B:47:ARG:CD	1:B:158:LEU:HD12	2.43	0.49
1:B:190:GLU:OE1	1:B:459:ARG:NH1	2.45	0.49
1:B:479:GLU:HB3	1:F:174:MET:HE1	1.95	0.49
1:F:248:LYS:HG2	1:F:252:LEU:HD21	1.94	0.49
1:F:443:PHE:CD2	1:F:470:ILE:HD13	2.48	0.49
1:A:390:ARG:HG2	1:A:390:ARG:HH11	1.78	0.49
1:B:204:PHE:CD2	1:B:468:VAL:HG21	2.48	0.49
1:E:204:PHE:CD2	1:E:468:VAL:HG21	2.48	0.49
1:E:212:PRO:CD	1:E:343:PRO:HG3	2.41	0.49
1:F:51:TYR:O	1:F:52:GLY:O	2.30	0.49
1:D:29:VAL:O	1:D:30:LEU:HD23	2.12	0.49
1:D:187:TYR:O	1:D:188:ARG:HD3	2.13	0.49
1:A:354:GLU:OE1	1:A:358:ARG:NH1	2.46	0.49
1:D:345:MET:HE2	1:D:380:GLU:CG	2.42	0.49
1:E:364:ILE:HB	1:E:440:LEU:HD23	1.95	0.49
1:A:10:PRO:HG2	1:B:461:GLY:HA3	1.94	0.48
1:A:291:THR:CG2	1:A:292:GLN:HE21	2.26	0.48
1:A:482:TYR:C	1:A:482:TYR:CD2	2.91	0.48
1:B:392:VAL:HG23	1:B:426:THR:CG2	2.42	0.48
1:E:443:PHE:CD2	1:E:470:ILE:HD13	2.48	0.48
1:F:73:ARG:HG2	1:F:83:ILE:HG21	1.95	0.48
1:A:437:GLU:O	1:A:437:GLU:HG2	2.13	0.48
1:B:1:MET:CE	1:B:4:ARG:HA	2.43	0.48
1:C:29:VAL:HB	1:C:187:TYR:CD2	2.46	0.48
1:C:124:GLU:HA	1:C:154:ALA:HA	1.95	0.48
1:D:61:THR:O	1:D:65:VAL:HG23	2.13	0.48
1:F:98:ALA:HA	1:F:101:ARG:NH1	2.29	0.48
1:F:354:GLU:OE1	1:F:358:ARG:NH1	2.46	0.48
1:F:391:PHE:HE2	1:F:408:GLN:HE21	1.61	0.48
1:B:8:ILE:CD1	1:B:75:LEU:CD1	2.89	0.48
1:B:441:VAL:HG13	1:B:465:PRO:HB3	1.96	0.48
1:B:486:ARG:HH11	1:B:486:ARG:HA	1.77	0.48
1:C:97:LYS:O	1:C:100:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LEU:HB3	1:C:286:ILE:CD1	2.42	0.48
1:C:462:ARG:HD2	1:F:6:ASP:HB3	1.94	0.48
1:D:109:PRO:HB2	1:D:142:ALA:HB3	1.94	0.48
1:E:287:GLU:O	1:E:291:THR:HB	2.14	0.48
1:A:253:ARG:NH1	1:A:257:ILE:HG12	2.27	0.48
1:D:291:THR:CG2	1:D:292:GLN:HE21	2.27	0.48
1:D:316:SER:O	1:D:320:PHE:HD1	1.96	0.48
1:F:169:THR:CG2	1:F:172:LYS:H	2.16	0.48
1:B:51:TYR:O	1:B:52:GLY:O	2.32	0.48
1:D:349:LYS:O	1:D:353:ARG:HD3	2.14	0.48
1:A:5:ARG:HD3	1:B:461:GLY:O	2.13	0.48
1:A:123:LEU:HD23	1:A:123:LEU:N	2.11	0.48
1:B:124:GLU:HB3	1:B:153:GLN:O	2.13	0.48
1:B:458:GLY:CA	1:B:464:MET:HE1	2.41	0.48
1:D:1:MET:HE2	1:D:4:ARG:CA	2.42	0.48
1:B:48:LEU:HD21	1:B:55:VAL:HG23	1.96	0.48
1:B:291:THR:CG2	1:B:292:GLN:HE21	2.27	0.48
1:B:464:MET:HG3	1:B:465:PRO:HD2	1.96	0.48
1:C:486:ARG:NH1	1:C:486:ARG:CA	2.77	0.48
1:D:248:LYS:HG2	1:D:252:LEU:HD21	1.96	0.48
1:F:124:GLU:O	1:F:155:LYS:HG3	2.14	0.48
1:A:207:VAL:CG2	1:A:471:LEU:HD23	2.43	0.48
1:B:323:LYS:O	1:B:326:LYS:HB2	2.14	0.48
1:C:124:GLU:HB3	1:C:153:GLN:O	2.14	0.48
1:C:174:MET:HE3	1:D:480:ALA:N	2.29	0.48
1:D:190:GLU:OE1	1:D:459:ARG:HD2	2.14	0.48
1:D:268:ASP:C	1:D:270:ARG:H	2.21	0.48
1:D:364:ILE:CG1	1:D:422:VAL:HG22	2.44	0.48
1:E:391:PHE:C	1:E:391:PHE:CD2	2.91	0.48
1:F:210:ASP:HA	1:F:474:LYS:HE2	1.95	0.48
1:F:364:ILE:HD12	1:F:364:ILE:C	2.39	0.48
1:A:204:PHE:HD2	1:A:468:VAL:HG21	1.79	0.48
1:B:37:THR:O	1:B:41:MET:HG3	2.14	0.48
1:A:364:ILE:HD11	1:A:366:VAL:HG23	1.96	0.48
1:A:443:PHE:HB3	1:A:445:GLU:O	2.14	0.48
1:B:443:PHE:CD2	1:B:470:ILE:HD13	2.49	0.48
1:C:128:LEU:HD13	1:C:158:LEU:HD13	1.94	0.48
1:D:34:LEU:CG	1:D:459:ARG:HG2	2.44	0.48
1:D:50:LYS:HD3	1:D:51:TYR:CZ	2.48	0.48
1:E:268:ASP:C	1:E:270:ARG:H	2.22	0.48
1:B:253:ARG:NH1	1:B:257:ILE:HG12	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:MET:HE2	1:B:380:GLU:HG2	1.96	0.47
1:C:58:LEU:HD12	1:C:131:PHE:CE2	2.49	0.47
1:C:243:SER:C	1:C:245:ASP:H	2.22	0.47
1:A:333:VAL:HG13	1:A:334:GLN:N	2.29	0.47
1:B:276:HIS:CE1	1:B:280:LEU:HD22	2.49	0.47
1:B:437:GLU:O	1:B:437:GLU:HG2	2.14	0.47
1:D:50:LYS:HD3	1:D:51:TYR:CE1	2.49	0.47
1:A:443:PHE:CD2	1:A:470:ILE:HD13	2.49	0.47
1:C:261:GLU:OE1	1:C:261:GLU:HA	2.12	0.47
1:D:354:GLU:O	1:D:358:ARG:HG3	2.15	0.47
1:E:243:SER:C	1:E:245:ASP:H	2.22	0.47
1:E:354:GLU:O	1:E:358:ARG:HG3	2.14	0.47
1:F:169:THR:HG23	1:F:171:GLU:OE2	2.14	0.47
1:A:1:MET:HE2	1:B:462:ARG:CZ	2.44	0.47
1:B:6:ASP:OD2	1:B:7:LEU:N	2.48	0.47
1:B:390:ARG:HG2	1:B:390:ARG:HH11	1.79	0.47
1:D:124:GLU:HA	1:D:154:ALA:HA	1.97	0.47
1:E:3:LEU:HD13	1:E:76:PHE:CE1	2.49	0.47
1:E:354:GLU:OE1	1:E:358:ARG:NH1	2.46	0.47
1:F:133:GLU:O	1:F:136:ARG:HG2	2.15	0.47
1:A:268:ASP:C	1:A:270:ARG:H	2.22	0.47
1:A:316:SER:O	1:A:320:PHE:HD1	1.98	0.47
1:B:187:TYR:O	1:B:188:ARG:HD3	2.15	0.47
1:B:480:ALA:CA	1:F:174:MET:HE3	2.43	0.47
1:E:105:ILE:HD12	1:E:105:ILE:C	2.39	0.47
1:F:366:VAL:HG22	1:F:442:VAL:CG1	2.45	0.47
1:B:6:ASP:OD2	1:B:7:LEU:HG	2.15	0.47
1:C:231:LYS:O	1:C:235:GLU:HG3	2.15	0.47
1:D:133:GLU:O	1:D:136:ARG:HG2	2.14	0.47
1:D:365:ILE:O	1:D:441:VAL:HA	2.15	0.47
1:F:109:PRO:HB2	1:F:142:ALA:HB3	1.97	0.47
1:A:122:SER:OG	1:A:124:GLU:HG3	2.15	0.47
1:A:260:GLU:O	1:A:264:LYS:HG3	2.14	0.47
1:A:266:ASN:HD22	1:A:266:ASN:HA	1.51	0.47
1:A:281:LYS:HE2	1:A:316:SER:OG	2.14	0.47
1:B:1:MET:HE3	1:B:5:ARG:N	2.28	0.47
1:B:29:VAL:O	1:B:30:LEU:HD23	2.14	0.47
1:B:109:PRO:HB2	1:B:142:ALA:HB3	1.96	0.47
1:B:206:TRP:CG	1:B:482:TYR:HD2	2.33	0.47
1:B:243:SER:C	1:B:245:ASP:H	2.23	0.47
1:C:51:TYR:O	1:C:52:GLY:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:GLU:O	1:C:291:THR:HB	2.15	0.47
1:E:25:ASN:ND2	1:E:159:VAL:H	2.12	0.47
1:E:124:GLU:HA	1:E:154:ALA:HA	1.97	0.47
1:E:169:THR:CG2	1:E:171:GLU:HB2	2.44	0.47
1:E:316:SER:O	1:E:320:PHE:HD1	1.97	0.47
1:E:374:ALA:O	1:E:378:VAL:HG23	2.13	0.47
1:E:390:ARG:HG2	1:E:390:ARG:NH1	2.29	0.47
1:F:349:LYS:HE3	1:F:380:GLU:HG3	1.97	0.47
1:A:97:LYS:O	1:A:100:ALA:HB3	2.14	0.47
1:B:374:ALA:O	1:B:378:VAL:HG23	2.15	0.47
1:E:228:ASP:HA	1:E:231:LYS:HD2	1.96	0.47
1:F:105:ILE:HD12	1:F:105:ILE:C	2.39	0.47
1:F:107:ALA:HB3	1:F:112:ILE:HD13	1.97	0.47
1:F:124:GLU:HA	1:F:154:ALA:HA	1.96	0.47
1:A:25:ASN:ND2	1:A:159:VAL:H	2.13	0.47
1:C:268:ASP:C	1:C:270:ARG:H	2.22	0.47
1:D:62:LYS:H	1:D:63:PRO:HD2	1.78	0.47
1:E:8:ILE:CD1	1:E:75:LEU:HD13	2.44	0.47
1:F:8:ILE:CG2	1:F:75:LEU:HD22	2.45	0.47
1:F:364:ILE:HG13	1:F:422:VAL:HG22	1.97	0.47
1:B:174:MET:HE3	1:F:480:ALA:CA	2.45	0.47
1:B:261:GLU:OE1	1:B:264:LYS:HD2	2.14	0.47
1:B:281:LYS:HD3	1:B:304:LEU:HD11	1.96	0.47
1:C:50:LYS:HD3	1:C:51:TYR:CE1	2.50	0.47
1:D:83:ILE:HD13	1:D:104:VAL:HB	1.96	0.47
1:D:248:LYS:HG2	1:D:252:LEU:CD2	2.45	0.47
1:E:78:LEU:O	1:E:79:PRO:C	2.59	0.47
1:F:342:HIS:CD2	1:F:343:PRO:HD2	2.50	0.47
1:F:373:THR:O	1:F:377:ILE:HG13	2.15	0.47
1:E:380:GLU:OE1	1:E:383:LYS:HD3	2.15	0.46
1:F:27:LEU:HD13	1:F:182:ILE:HG13	1.96	0.46
1:F:56:LEU:HD13	1:F:105:ILE:HG13	1.96	0.46
1:F:58:LEU:HA	1:F:107:ALA:O	2.15	0.46
1:F:62:LYS:HE3	1:F:89:GLU:OE1	2.15	0.46
1:F:287:GLU:O	1:F:291:THR:HB	2.15	0.46
1:A:98:ALA:HA	1:A:101:ARG:NH1	2.30	0.46
1:A:150:TYR:OH	1:A:157:PRO:HA	2.15	0.46
1:B:313:THR:HG22	1:B:315:ALA:H	1.81	0.46
1:C:342:HIS:CD2	1:C:343:PRO:HD2	2.50	0.46
1:D:1:MET:HE2	1:D:5:ARG:N	2.30	0.46
1:D:124:GLU:HB3	1:D:153:GLN:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:PHE:CD2	1:D:470:ILE:HD13	2.50	0.46
1:A:2:VAL:HB	1:A:45:GLU:HG3	1.97	0.46
1:B:62:LYS:H	1:B:63:PRO:HD2	1.80	0.46
1:B:226:LEU:HD22	1:B:230:LEU:CD1	2.45	0.46
1:B:472:MET:O	1:B:472:MET:HG3	2.15	0.46
1:C:354:GLU:OE1	1:C:358:ARG:NH1	2.48	0.46
1:D:225:MET:HE1	1:D:325:MET:HB2	1.97	0.46
1:D:287:GLU:O	1:D:291:THR:HB	2.15	0.46
1:F:11:ARG:NH2	1:F:459:ARG:O	2.48	0.46
1:A:47:ARG:NH2	1:A:158:LEU:HB2	2.30	0.46
1:A:204:PHE:CD2	1:A:468:VAL:HG21	2.51	0.46
1:D:462:ARG:HE	1:E:1:MET:HE3	1.80	0.46
1:D:464:MET:HE2	1:D:464:MET:HB2	1.87	0.46
1:E:109:PRO:HB2	1:E:142:ALA:HB3	1.97	0.46
1:E:365:ILE:O	1:E:441:VAL:HA	2.15	0.46
1:E:392:VAL:HG13	1:E:408:GLN:NE2	2.29	0.46
1:F:281:LYS:CD	1:F:304:LEU:HD11	2.45	0.46
1:C:55:VAL:HG13	1:C:128:LEU:HD23	1.97	0.46
1:C:107:ALA:HB3	1:C:112:ILE:HD13	1.98	0.46
1:C:204:PHE:CD2	1:C:468:VAL:HG21	2.50	0.46
1:C:363:LYS:HD3	1:C:437:GLU:O	2.16	0.46
1:E:56:LEU:HD13	1:E:105:ILE:HG13	1.97	0.46
1:E:190:GLU:OE1	1:E:459:ARG:NH1	2.45	0.46
1:E:291:THR:CG2	1:E:292:GLN:HE21	2.28	0.46
1:F:236:THR:HG21	1:F:269:LEU:HD22	1.97	0.46
1:A:169:THR:HG22	1:A:171:GLU:N	2.30	0.46
1:C:124:GLU:O	1:C:155:LYS:HG3	2.15	0.46
1:D:184:HIS:HE1	1:D:186:GLU:OE2	1.99	0.46
1:D:281:LYS:CD	1:D:304:LEU:HD11	2.46	0.46
1:D:454:ILE:HA	1:D:457:ARG:CG	2.46	0.46
1:D:458:GLY:CA	1:D:464:MET:HE1	2.36	0.46
1:E:477:ARG:O	1:E:478:ASP:C	2.58	0.46
1:F:351:ILE:HG13	1:F:352:ILE:N	2.30	0.46
1:C:364:ILE:HD12	1:C:364:ILE:C	2.41	0.46
1:D:390:ARG:HG3	1:D:391:PHE:N	2.31	0.46
1:F:58:LEU:HD12	1:F:131:PHE:CE2	2.51	0.46
1:F:266:ASN:HD22	1:F:266:ASN:HA	1.52	0.46
1:F:291:THR:CG2	1:F:292:GLN:HE21	2.29	0.46
1:A:225:MET:HG2	1:A:324:ARG:HH21	1.81	0.46
1:C:105:ILE:HD12	1:C:105:ILE:C	2.41	0.46
1:C:109:PRO:HB2	1:C:142:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:LYS:HE3	1:D:380:GLU:HG3	1.97	0.46
1:B:185:ILE:CG2	1:B:187:TYR:CE1	2.99	0.46
1:D:32:THR:CG2	1:D:456:ARG:HD3	2.46	0.46
1:E:426:THR:CG2	1:E:428:VAL:HG12	2.31	0.46
1:F:187:TYR:O	1:F:188:ARG:HD3	2.15	0.46
1:F:316:SER:O	1:F:320:PHE:HD1	1.98	0.46
1:A:364:ILE:HG13	1:A:422:VAL:HG22	1.98	0.46
1:A:472:MET:CE	1:A:479:GLU:HA	2.45	0.46
1:A:480:ALA:N	1:E:174:MET:HE3	2.30	0.46
1:B:365:ILE:O	1:B:441:VAL:HA	2.16	0.46
1:D:174:MET:CE	1:D:177:ILE:HD12	2.46	0.46
1:E:351:ILE:HG13	1:E:352:ILE:N	2.30	0.46
1:F:11:ARG:HB3	1:F:198:TYR:CZ	2.51	0.46
1:F:389:LYS:HD3	1:F:420:PHE:CE2	2.51	0.46
1:A:1:MET:CE	1:B:462:ARG:CZ	2.94	0.45
1:A:60:PRO:HG3	1:A:136:ARG:HD3	1.98	0.45
1:A:105:ILE:HD11	1:A:107:ALA:HB2	1.97	0.45
1:A:406:ARG:HB3	1:A:406:ARG:HH11	1.77	0.45
1:A:480:ALA:H	1:E:174:MET:HE3	1.80	0.45
1:B:60:PRO:HB3	1:B:136:ARG:CZ	2.46	0.45
1:C:351:ILE:HG13	1:C:352:ILE:N	2.31	0.45
1:C:354:GLU:O	1:C:358:ARG:HG3	2.16	0.45
1:E:281:LYS:CD	1:E:304:LEU:HD11	2.46	0.45
1:F:11:ARG:N	1:F:14:GLN:HE21	2.03	0.45
1:F:60:PRO:HB3	1:F:136:ARG:CZ	2.46	0.45
1:F:391:PHE:C	1:F:391:PHE:HD2	2.22	0.45
1:A:243:SER:C	1:A:245:ASP:H	2.24	0.45
1:A:276:HIS:CE1	1:A:280:LEU:HD22	2.51	0.45
1:A:354:GLU:O	1:A:358:ARG:HG3	2.16	0.45
1:A:394:GLN:CG	1:A:405:GLN:N	2.79	0.45
1:B:241:SER:HB3	1:F:139:GLY:CA	2.46	0.45
1:E:391:PHE:HB3	1:E:425:ALA:HB2	1.97	0.45
1:B:391:PHE:C	1:B:391:PHE:HD2	2.24	0.45
1:B:457:ARG:HG2	1:B:457:ARG:H	1.55	0.45
1:D:9:GLN:HB3	1:E:11:ARG:NH1	2.31	0.45
1:F:30:LEU:HD22	1:F:188:ARG:HB3	1.97	0.45
1:F:392:VAL:HG13	1:F:408:GLN:HE21	1.81	0.45
1:B:124:GLU:HA	1:B:154:ALA:HA	1.99	0.45
1:B:342:HIS:CD2	1:B:343:PRO:HD2	2.52	0.45
1:B:380:GLU:OE1	1:B:383:LYS:HD3	2.17	0.45
1:B:392:VAL:HG23	1:B:426:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:THR:O	1:C:65:VAL:HG23	2.15	0.45
1:C:345:MET:HE2	1:C:380:GLU:HG2	1.99	0.45
1:E:230:LEU:HD22	1:E:239:LEU:HD11	1.99	0.45
1:F:354:GLU:O	1:F:358:ARG:HG3	2.16	0.45
1:B:393:GLY:N	1:B:428:VAL:HG11	2.32	0.45
1:D:266:ASN:HD22	1:D:266:ASN:HA	1.51	0.45
1:D:273:LEU:HD12	1:D:273:LEU:HA	1.83	0.45
1:A:113:GLU:HG3	1:A:145:PHE:CD2	2.52	0.45
1:B:47:ARG:NH2	1:B:158:LEU:HB2	2.31	0.45
1:B:50:LYS:HD3	1:B:51:TYR:CE1	2.51	0.45
1:C:187:TYR:O	1:C:188:ARG:HD3	2.17	0.45
1:D:302:LYS:HE2	1:D:302:LYS:HB3	1.76	0.45
1:D:342:HIS:CD2	1:D:344:LYS:H	2.27	0.45
1:E:124:GLU:H	1:E:124:GLU:HG3	1.64	0.45
1:F:434:ASP:OD1	1:F:462:ARG:NH2	2.48	0.45
1:C:30:LEU:HD22	1:C:188:ARG:HB3	1.98	0.45
1:C:255:GLY:HA3	1:C:276:HIS:NE2	2.32	0.45
1:B:364:ILE:HB	1:B:440:LEU:HD23	1.98	0.45
1:B:479:GLU:HG2	1:B:483:TRP:NE1	2.32	0.45
1:D:473:ALA:HB3	1:D:476:THR:CG2	2.45	0.45
1:E:98:ALA:HA	1:E:101:ARG:NH1	2.32	0.45
1:B:169:THR:HG23	1:B:171:GLU:OE2	2.17	0.45
1:C:291:THR:HG22	1:C:292:GLN:HE21	1.82	0.45
1:D:105:ILE:HD11	1:D:107:ALA:HB2	1.99	0.45
1:D:248:LYS:O	1:D:252:LEU:HD22	2.17	0.45
1:E:124:GLU:HB3	1:E:153:GLN:O	2.17	0.45
1:F:364:ILE:CD1	1:F:366:VAL:HG23	2.47	0.45
1:F:437:GLU:O	1:F:437:GLU:HG2	2.17	0.45
1:A:48:LEU:HD21	1:A:55:VAL:HG23	1.98	0.45
1:A:472:MET:HE1	1:A:482:TYR:CB	2.46	0.45
1:C:45:GLU:OE1	1:F:463:HIS:HE1	2.00	0.45
1:C:60:PRO:HG3	1:C:136:ARG:HD3	1.98	0.45
1:C:349:LYS:O	1:C:353:ARG:HD3	2.17	0.45
1:D:17:ILE:O	1:D:18:TYR:C	2.59	0.45
1:E:231:LYS:N	1:E:232:PRO:HD2	2.32	0.45
1:E:253:ARG:NH1	1:E:257:ILE:HG12	2.32	0.45
1:E:443:PHE:HB3	1:E:445:GLU:O	2.17	0.45
1:F:56:LEU:CD1	1:F:105:ILE:HG13	2.47	0.45
1:F:219:ARG:NE	1:F:290:GLU:OE1	2.45	0.45
1:F:253:ARG:O	1:F:257:ILE:HG13	2.17	0.45
1:A:29:VAL:O	1:A:30:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TRP:C	1:A:485:SER:H	2.25	0.44
1:B:174:MET:HE2	1:B:177:ILE:HD12	1.99	0.44
1:B:241:SER:CB	1:F:139:GLY:CA	2.92	0.44
1:B:454:ILE:HA	1:B:457:ARG:CG	2.47	0.44
1:C:364:ILE:HD11	1:C:366:VAL:HG23	1.97	0.44
1:E:391:PHE:HB2	1:E:423:LEU:CD1	2.40	0.44
1:E:477:ARG:HB3	1:E:477:ARG:CZ	2.43	0.44
1:E:477:ARG:CB	1:E:477:ARG:CZ	2.95	0.44
1:B:392:VAL:HG13	1:B:393:GLY:N	2.31	0.44
1:C:281:LYS:CD	1:C:304:LEU:HD11	2.45	0.44
1:C:365:ILE:O	1:C:441:VAL:HA	2.17	0.44
1:D:333:VAL:CG1	1:D:334:GLN:N	2.80	0.44
1:E:457:ARG:HG2	1:E:457:ARG:H	1.64	0.44
1:F:289:LEU:HD13	1:F:294:LEU:HD23	1.99	0.44
1:F:380:GLU:OE1	1:F:383:LYS:HD3	2.16	0.44
1:B:355:GLN:NE2	1:B:358:ARG:HH22	2.15	0.44
1:C:48:LEU:HD21	1:C:55:VAL:HG23	1.99	0.44
1:D:60:PRO:HG3	1:D:136:ARG:HD3	1.99	0.44
1:A:405:GLN:N	1:A:408:GLN:HG3	2.32	0.44
1:A:473:ALA:O	1:A:474:LYS:C	2.60	0.44
1:B:174:MET:CE	1:B:177:ILE:HD12	2.46	0.44
1:B:354:GLU:O	1:B:358:ARG:HG3	2.17	0.44
1:C:302:LYS:O	1:C:305:TYR:N	2.46	0.44
1:D:258:ILE:CG2	1:D:273:LEU:HD13	2.39	0.44
1:E:122:SER:OG	1:E:124:GLU:CG	2.65	0.44
1:B:1:MET:HE3	1:B:4:ARG:HA	1.99	0.44
1:C:476:THR:O	1:D:174:MET:SD	2.76	0.44
1:D:30:LEU:CD2	1:D:188:ARG:CB	2.96	0.44
1:D:56:LEU:HD13	1:D:105:ILE:HG13	2.00	0.44
1:D:60:PRO:HB3	1:D:136:ARG:CZ	2.47	0.44
1:D:441:VAL:HG13	1:D:465:PRO:HB3	1.99	0.44
1:F:405:GLN:N	1:F:407:GLU:OE1	2.50	0.44
1:C:75:LEU:HD11	1:F:7:LEU:HD22	2.00	0.44
1:D:364:ILE:HD11	1:D:366:VAL:HG23	2.00	0.44
1:E:11:ARG:NH2	1:E:459:ARG:O	2.51	0.44
1:F:105:ILE:HD11	1:F:107:ALA:HB2	1.98	0.44
1:F:226:LEU:HD22	1:F:230:LEU:CD1	2.48	0.44
1:F:309:LYS:C	1:F:311:GLY:N	2.72	0.44
1:A:483:TRP:O	1:A:484:SER:C	2.60	0.44
1:B:8:ILE:HD12	1:B:38:LEU:HD22	2.00	0.44
1:C:454:ILE:HA	1:C:457:ARG:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:PHE:HA	1:D:468:VAL:HG22	2.00	0.44
1:D:207:VAL:HG13	1:D:469:ILE:HG23	2.00	0.44
1:F:438:VAL:O	1:F:438:VAL:HG22	2.18	0.44
1:C:56:LEU:CD1	1:C:105:ILE:HG13	2.48	0.44
1:C:345:MET:CA	1:C:345:MET:HE3	2.48	0.44
1:D:22:LYS:CG	1:D:46:TYR:CD2	3.00	0.44
1:D:105:ILE:HD12	1:D:105:ILE:C	2.42	0.44
1:D:185:ILE:HG21	1:D:187:TYR:CE1	2.52	0.44
1:E:236:THR:HG21	1:E:269:LEU:HD22	2.00	0.44
1:E:273:LEU:HD12	1:E:273:LEU:HA	1.86	0.44
1:E:487:GLN:O	1:E:487:GLN:HG2	2.17	0.44
1:F:323:LYS:O	1:F:326:LYS:HB2	2.18	0.44
1:F:345:MET:CA	1:F:345:MET:HE3	2.48	0.44
1:A:27:LEU:HD13	1:A:182:ILE:HG13	1.99	0.44
1:B:69:ALA:O	1:B:73:ARG:HG3	2.18	0.44
1:B:440:LEU:HG	1:B:441:VAL:N	2.32	0.44
1:C:441:VAL:HG13	1:C:465:PRO:HB3	2.00	0.44
1:E:2:VAL:HB	1:E:45:GLU:HG3	1.99	0.44
1:E:60:PRO:HG3	1:E:136:ARG:HD3	2.00	0.44
1:E:322:ASP:OD2	1:E:324:ARG:HB2	2.17	0.44
1:A:22:LYS:HD2	1:A:46:TYR:CD1	2.53	0.43
1:A:124:GLU:HA	1:A:153:GLN:O	2.18	0.43
1:B:3:LEU:HD12	1:B:42:MET:HA	2.00	0.43
1:B:105:ILE:HD11	1:B:107:ALA:HB2	1.98	0.43
1:D:9:GLN:HB3	1:E:11:ARG:HH11	1.82	0.43
1:D:51:TYR:O	1:D:52:GLY:O	2.35	0.43
1:E:248:LYS:O	1:E:252:LEU:HD22	2.18	0.43
1:D:22:LYS:HG3	1:D:46:TYR:CD2	2.53	0.43
1:D:123:LEU:CD2	1:D:123:LEU:N	2.73	0.43
1:E:113:GLU:HG3	1:E:145:PHE:CD2	2.53	0.43
1:E:345:MET:HE3	1:E:345:MET:O	2.18	0.43
1:F:30:LEU:CD2	1:F:188:ARG:HB2	2.48	0.43
1:B:236:THR:HG21	1:B:269:LEU:HD22	2.01	0.43
1:B:302:LYS:HB3	1:B:302:LYS:HE2	1.75	0.43
1:C:22:LYS:CG	1:C:46:TYR:CE2	2.99	0.43
1:D:456:ARG:HH11	1:D:456:ARG:CG	2.31	0.43
1:E:192:SER:C	1:E:194:ASP:N	2.76	0.43
1:E:225:MET:HG2	1:E:324:ARG:HH21	1.83	0.43
1:F:61:THR:O	1:F:65:VAL:HG23	2.19	0.43
1:A:486:ARG:HH22	1:E:165:SER:HA	1.84	0.43
1:F:43:ILE:O	1:F:47:ARG:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ALA:HB3	1:D:112:ILE:HD13	2.00	0.43
1:E:22:LYS:HD2	1:E:46:TYR:CE1	2.54	0.43
1:B:133:GLU:O	1:B:136:ARG:HG2	2.19	0.43
1:C:60:PRO:HB3	1:C:136:ARG:CZ	2.49	0.43
1:C:190:GLU:HG3	1:C:199:VAL:HG11	2.01	0.43
1:C:289:LEU:HD13	1:C:294:LEU:HD23	2.01	0.43
1:D:112:ILE:CG2	1:D:146:ILE:HD13	2.48	0.43
1:B:210:ASP:CA	1:B:474:LYS:HE3	2.43	0.43
1:C:349:LYS:HE3	1:C:380:GLU:HG3	2.00	0.43
1:C:366:VAL:HG22	1:C:442:VAL:HG13	2.00	0.43
1:D:174:MET:HE2	1:D:177:ILE:HD12	2.01	0.43
1:D:236:THR:HG21	1:D:269:LEU:HD22	2.01	0.43
1:E:133:GLU:OE1	1:E:136:ARG:NH1	2.46	0.43
1:F:30:LEU:CD2	1:F:188:ARG:CB	2.96	0.43
1:A:22:LYS:HG3	1:A:46:TYR:CD2	2.54	0.43
1:B:266:ASN:O	1:B:267:HIS:HB2	2.19	0.43
1:C:22:LYS:HG3	1:C:46:TYR:CD2	2.54	0.43
1:C:73:ARG:HG2	1:C:83:ILE:HG21	2.01	0.43
1:C:266:ASN:O	1:C:267:HIS:HB2	2.18	0.43
1:E:35:GLY:O	1:E:36:LYS:C	2.61	0.43
1:E:128:LEU:HD13	1:E:158:LEU:HD13	2.00	0.43
1:E:261:GLU:OE1	1:E:261:GLU:HA	2.19	0.43
1:F:35:GLY:O	1:F:36:LYS:C	2.61	0.43
1:F:62:LYS:H	1:F:63:PRO:HD2	1.83	0.43
1:F:204:PHE:HA	1:F:468:VAL:HG22	2.00	0.43
1:A:124:GLU:HB3	1:A:153:GLN:O	2.19	0.43
1:A:261:GLU:OE1	1:A:264:LYS:HD2	2.18	0.43
1:A:457:ARG:HG2	1:A:457:ARG:H	1.66	0.43
1:B:192:SER:C	1:B:194:ASP:N	2.76	0.43
1:C:4:ARG:HA	1:C:4:ARG:HD2	1.88	0.43
1:C:41:MET:HE2	1:C:72:PHE:HA	2.01	0.43
1:D:124:GLU:O	1:D:155:LYS:HG3	2.19	0.43
1:E:344:LYS:NZ	1:E:478:ASP:OD1	2.39	0.43
1:A:5:ARG:NH1	1:A:15:GLU:OE2	2.45	0.43
1:A:10:PRO:HA	1:A:14:GLN:NE2	2.34	0.43
1:A:454:ILE:HA	1:A:457:ARG:CG	2.49	0.43
1:B:8:ILE:CD1	1:B:75:LEU:HD22	2.49	0.43
1:B:211:LEU:HB2	1:B:474:LYS:NZ	2.34	0.43
1:C:105:ILE:HD11	1:C:107:ALA:HB2	2.01	0.43
1:C:150:TYR:OH	1:C:157:PRO:HA	2.19	0.43
1:D:116:LEU:HD12	1:D:116:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:LYS:N	1:D:232:PRO:HD2	2.33	0.43
1:E:83:ILE:HD13	1:E:104:VAL:HB	2.01	0.43
1:A:22:LYS:HG2	1:A:46:TYR:CE2	2.54	0.42
1:A:72:PHE:O	1:A:76:PHE:HB2	2.19	0.42
1:A:248:LYS:O	1:A:252:LEU:HD22	2.19	0.42
1:B:202:ILE:HG21	1:B:204:PHE:CZ	2.54	0.42
1:B:222:LEU:CB	1:B:286:ILE:HD13	2.49	0.42
1:B:454:ILE:HA	1:B:457:ARG:HG3	2.00	0.42
1:E:364:ILE:HD11	1:E:366:VAL:HG23	2.01	0.42
1:B:248:LYS:HG2	1:B:252:LEU:HD21	2.00	0.42
1:C:8:ILE:CG1	1:C:10:PRO:HD3	2.49	0.42
1:C:29:VAL:O	1:C:30:LEU:HD23	2.18	0.42
1:C:124:GLU:HA	1:C:153:GLN:O	2.19	0.42
1:C:174:MET:HE2	1:C:177:ILE:HD12	2.00	0.42
1:F:273:LEU:HD12	1:F:273:LEU:HA	1.88	0.42
1:A:61:THR:HB	1:A:63:PRO:HD2	2.00	0.42
1:B:261:GLU:OE1	1:B:261:GLU:HA	2.20	0.42
1:B:291:THR:HG23	1:B:373:THR:OG1	2.19	0.42
1:C:192:SER:C	1:C:194:ASP:N	2.75	0.42
1:C:261:GLU:OE1	1:C:264:LYS:HD2	2.19	0.42
1:C:289:LEU:CD1	1:C:294:LEU:HD23	2.49	0.42
1:C:380:GLU:OE1	1:C:383:LYS:HD3	2.19	0.42
1:D:11:ARG:N	1:D:14:GLN:HE21	2.09	0.42
1:E:116:LEU:HD12	1:E:116:LEU:HA	1.82	0.42
1:F:47:ARG:CD	1:F:158:LEU:HD12	2.48	0.42
1:F:83:ILE:HD13	1:F:104:VAL:HB	2.01	0.42
1:F:212:PRO:HD2	1:F:343:PRO:HG2	2.00	0.42
1:A:56:LEU:HD13	1:A:105:ILE:HG13	2.00	0.42
1:A:426:THR:CG2	1:A:428:VAL:HG12	2.35	0.42
1:A:452:ARG:HD2	1:A:456:ARG:NH2	2.34	0.42
1:B:140:ASN:HD22	1:B:140:ASN:HA	1.61	0.42
1:B:390:ARG:HG3	1:B:391:PHE:N	2.34	0.42
1:E:441:VAL:HG13	1:E:465:PRO:HB3	2.00	0.42
1:E:452:ARG:HD2	1:E:456:ARG:NH2	2.34	0.42
1:F:192:SER:C	1:F:194:ASP:N	2.75	0.42
1:F:261:GLU:OE1	1:F:261:GLU:HA	2.18	0.42
1:A:8:ILE:HG23	1:A:75:LEU:HD22	2.01	0.42
1:B:105:ILE:HD12	1:B:105:ILE:C	2.44	0.42
1:B:243:SER:C	1:B:245:ASP:N	2.77	0.42
1:B:333:VAL:CG1	1:B:334:GLN:N	2.82	0.42
1:C:16:VAL:O	1:C:19:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ARG:CD	1:C:158:LEU:HD12	2.49	0.42
1:C:236:THR:HG21	1:C:269:LEU:HD22	2.00	0.42
1:C:443:PHE:HE1	1:C:450:ALA:HB3	1.84	0.42
1:E:390:ARG:HG2	1:E:390:ARG:HH11	1.84	0.42
1:F:55:VAL:HG13	1:F:128:LEU:HD23	2.02	0.42
1:F:128:LEU:HD13	1:F:158:LEU:HD13	2.01	0.42
1:F:208:ARG:HD3	1:F:474:LYS:CG	2.49	0.42
1:F:211:LEU:HD22	1:F:215:TYR:CD2	2.54	0.42
1:F:253:ARG:NH1	1:F:257:ILE:HG12	2.35	0.42
1:F:454:ILE:HA	1:F:457:ARG:CG	2.49	0.42
1:B:248:LYS:HG2	1:B:252:LEU:CD2	2.50	0.42
1:C:43:ILE:O	1:C:47:ARG:HG2	2.19	0.42
1:D:122:SER:OG	1:D:124:GLU:CG	2.68	0.42
1:D:223:ARG:NH2	1:D:245:ASP:OD1	2.53	0.42
1:D:389:LYS:HD3	1:D:420:PHE:CE2	2.55	0.42
1:E:323:LYS:O	1:E:326:LYS:HB2	2.18	0.42
1:F:116:LEU:HD12	1:F:116:LEU:HA	1.81	0.42
1:F:228:ASP:HA	1:F:231:LYS:HD2	2.00	0.42
1:D:294:LEU:HD12	1:D:340:LEU:O	2.19	0.42
1:D:380:GLU:OE1	1:D:383:LYS:HD3	2.20	0.42
1:E:266:ASN:HD22	1:E:266:ASN:HA	1.52	0.42
1:F:37:THR:O	1:F:40:ALA:HB3	2.20	0.42
1:F:169:THR:HG22	1:F:171:GLU:N	2.35	0.42
1:F:406:ARG:HH11	1:F:406:ARG:CA	2.30	0.42
1:A:11:ARG:N	1:A:14:GLN:HE21	2.13	0.42
1:A:78:LEU:O	1:A:79:PRO:C	2.63	0.42
1:A:463:HIS:HE1	1:B:45:GLU:OE1	2.02	0.42
1:B:22:LYS:HG3	1:B:46:TYR:CD2	2.55	0.42
1:B:364:ILE:HG13	1:B:422:VAL:HG22	2.01	0.42
1:D:98:ALA:HA	1:D:101:ARG:NH1	2.35	0.42
1:D:243:SER:C	1:D:245:ASP:N	2.77	0.42
1:E:179:ASN:HD22	1:E:179:ASN:HA	1.60	0.42
1:A:345:MET:HE2	1:A:380:GLU:CG	2.50	0.42
1:B:23:GLU:OE2	1:B:47:ARG:NH1	2.53	0.42
1:C:174:MET:HE3	1:D:480:ALA:HB2	2.01	0.42
1:C:255:GLY:CA	1:C:276:HIS:CD2	3.03	0.42
1:D:128:LEU:HD13	1:D:158:LEU:HD13	2.02	0.42
1:D:366:VAL:HG22	1:D:442:VAL:HG13	2.01	0.42
1:D:414:GLU:O	1:D:419:GLU:HB2	2.20	0.42
1:E:73:ARG:HG2	1:E:83:ILE:HG21	2.02	0.42
1:F:231:LYS:O	1:F:235:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:SER:OG	1:B:94:GLU:HG3	2.20	0.42
1:C:190:GLU:CG	1:C:199:VAL:HG11	2.50	0.42
1:D:354:GLU:OE1	1:D:358:ARG:NH1	2.53	0.42
1:E:61:THR:O	1:E:65:VAL:HG23	2.20	0.42
1:E:302:LYS:O	1:E:305:TYR:N	2.50	0.42
1:F:4:ARG:HA	1:F:4:ARG:HD2	1.83	0.42
1:F:302:LYS:O	1:F:305:TYR:N	2.51	0.42
1:B:349:LYS:O	1:B:353:ARG:HD3	2.19	0.41
1:C:342:HIS:HA	1:C:343:PRO:HD3	1.82	0.41
1:C:463:HIS:HE1	1:F:45:GLU:OE1	2.02	0.41
1:D:47:ARG:NH2	1:D:158:LEU:HB2	2.35	0.41
1:D:169:THR:HG22	1:D:171:GLU:N	2.34	0.41
1:D:302:LYS:O	1:D:305:TYR:N	2.46	0.41
1:D:412:LEU:HD12	1:D:412:LEU:HA	1.91	0.41
1:F:29:VAL:HB	1:F:187:TYR:CD2	2.54	0.41
1:A:4:ARG:HG3	1:A:4:ARG:HH11	1.85	0.41
1:A:12:ILE:HG13	1:A:198:TYR:OH	2.19	0.41
1:C:123:LEU:HD23	1:C:123:LEU:N	2.20	0.41
1:C:347:LYS:O	1:C:351:ILE:HG23	2.20	0.41
1:D:56:LEU:CD1	1:D:105:ILE:HG13	2.50	0.41
1:D:253:ARG:O	1:D:257:ILE:HG13	2.20	0.41
1:E:56:LEU:CD1	1:E:105:ILE:HG13	2.50	0.41
1:A:243:SER:C	1:A:245:ASP:N	2.78	0.41
1:A:273:LEU:HD12	1:A:273:LEU:HA	1.87	0.41
1:B:190:GLU:CG	1:B:199:VAL:HG11	2.50	0.41
1:C:185:ILE:HB	1:D:483:TRP:CE3	2.54	0.41
1:C:345:MET:HE3	1:C:345:MET:O	2.19	0.41
1:D:1:MET:HE1	1:D:6:ASP:N	2.31	0.41
1:D:58:LEU:HD12	1:D:131:PHE:CE2	2.55	0.41
1:E:276:HIS:CE1	1:E:280:LEU:HD22	2.55	0.41
1:E:437:GLU:O	1:E:437:GLU:HG2	2.20	0.41
1:A:36:LYS:N	2:A:495:PO4:O1	2.53	0.41
1:A:302:LYS:HE2	1:A:302:LYS:HB3	1.72	0.41
1:D:1:MET:HG3	1:D:3:LEU:O	2.21	0.41
1:D:34:LEU:HD21	1:D:459:ARG:HG2	2.03	0.41
1:D:41:MET:HE2	1:D:72:PHE:CD1	2.55	0.41
1:D:190:GLU:CG	1:D:199:VAL:HG11	2.50	0.41
1:D:281:LYS:HE2	1:D:316:SER:OG	2.20	0.41
1:D:351:ILE:HG13	1:D:352:ILE:N	2.36	0.41
1:E:123:LEU:CD2	1:E:123:LEU:N	2.79	0.41
1:E:345:MET:HE3	1:E:345:MET:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:LYS:N	1:F:63:PRO:CD	2.83	0.41
1:F:97:LYS:O	1:F:100:ALA:HB3	2.21	0.41
1:F:443:PHE:HE1	1:F:450:ALA:HB3	1.85	0.41
1:A:212:PRO:HD2	1:A:343:PRO:HG2	2.01	0.41
1:B:164:ALA:O	1:B:165:SER:HB2	2.20	0.41
1:C:62:LYS:H	1:C:63:PRO:HD2	1.85	0.41
1:C:130:VAL:HA	1:C:160:ILE:O	2.21	0.41
1:C:412:LEU:HD12	1:C:412:LEU:HA	1.93	0.41
1:E:150:TYR:OH	1:E:157:PRO:HA	2.20	0.41
1:F:69:ALA:O	1:F:73:ARG:HG3	2.20	0.41
1:F:248:LYS:HB2	1:F:283:HIS:CE1	2.55	0.41
1:A:62:LYS:HG3	1:A:63:PRO:HD2	1.99	0.41
1:A:349:LYS:O	1:A:353:ARG:HD3	2.21	0.41
1:A:351:ILE:HG13	1:A:352:ILE:N	2.35	0.41
1:B:112:ILE:CG2	1:B:146:ILE:HD13	2.50	0.41
1:B:169:THR:HG22	1:B:171:GLU:N	2.34	0.41
1:D:190:GLU:HG3	1:D:199:VAL:HG11	2.01	0.41
1:E:60:PRO:HB3	1:E:136:ARG:CZ	2.51	0.41
1:E:135:HIS:CD2	1:E:163:THR:OG1	2.74	0.41
1:F:344:LYS:HB3	1:F:444:TYR:CE2	2.54	0.41
1:A:380:GLU:OE1	1:A:383:LYS:HD3	2.20	0.41
1:B:176:VAL:HG23	1:B:180:LEU:HD12	2.02	0.41
1:B:364:ILE:HD11	1:B:366:VAL:HG23	2.03	0.41
1:C:2:VAL:HB	1:C:45:GLU:OE2	2.20	0.41
1:C:22:LYS:HD2	1:C:46:TYR:CE1	2.55	0.41
1:D:192:SER:C	1:D:194:ASP:N	2.77	0.41
1:D:333:VAL:HG13	1:D:334:GLN:N	2.35	0.41
1:D:351:ILE:HD12	1:D:469:ILE:HD12	2.02	0.41
1:E:11:ARG:N	1:E:14:GLN:HE21	2.15	0.41
1:E:169:THR:HG22	1:E:172:LYS:N	2.26	0.41
1:F:190:GLU:OE1	1:F:459:ARG:NH1	2.47	0.41
1:A:83:ILE:HD13	1:A:104:VAL:HB	2.02	0.41
1:A:190:GLU:CG	1:A:199:VAL:HG11	2.51	0.41
1:A:472:MET:CB	1:A:478:ASP:HB3	2.50	0.41
1:B:410:LEU:O	1:B:414:GLU:HG3	2.20	0.41
1:C:17:ILE:O	1:C:18:TYR:C	2.63	0.41
1:E:30:LEU:O	1:E:36:LYS:HE2	2.21	0.41
1:E:169:THR:CG2	1:E:171:GLU:OE2	2.67	0.41
1:E:190:GLU:CG	1:E:199:VAL:HG11	2.50	0.41
1:F:11:ARG:HD3	1:F:14:GLN:NE2	2.36	0.41
1:F:115:ASP:HA	1:F:120:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:MET:CE	1:F:177:ILE:HD12	2.51	0.41
1:A:211:LEU:HD22	1:A:215:TYR:CD2	2.56	0.41
1:A:349:LYS:HE3	1:A:380:GLU:HG3	2.03	0.41
1:A:443:PHE:HE1	1:A:450:ALA:HB3	1.86	0.41
1:B:316:SER:O	1:B:320:PHE:HD1	2.04	0.41
1:B:366:VAL:HG22	1:B:442:VAL:HG13	2.02	0.41
1:C:4:ARG:HE	1:C:6:ASP:CG	2.28	0.41
1:C:37:THR:O	1:C:41:MET:HG3	2.20	0.41
1:C:116:LEU:HD12	1:C:116:LEU:HA	1.83	0.41
1:C:223:ARG:HH22	1:C:245:ASP:CG	2.29	0.41
1:D:22:LYS:CG	1:D:46:TYR:CE2	2.99	0.41
1:D:22:LYS:HD2	1:D:46:TYR:CD1	2.55	0.41
1:D:41:MET:HE2	1:D:72:PHE:CG	2.56	0.41
1:D:221:LEU:HD22	1:D:324:ARG:HG2	2.03	0.41
1:D:266:ASN:O	1:D:267:HIS:HB2	2.21	0.41
1:D:342:HIS:HA	1:D:343:PRO:HD3	1.91	0.41
1:D:364:ILE:HG13	1:D:422:VAL:HG22	2.02	0.41
1:D:454:ILE:HA	1:D:457:ARG:HG3	2.01	0.41
1:D:462:ARG:HE	1:E:1:MET:CE	2.33	0.41
1:E:17:ILE:O	1:E:18:TYR:C	2.64	0.41
1:E:364:ILE:CD1	1:E:366:VAL:HG23	2.51	0.41
1:E:389:LYS:HD3	1:E:420:PHE:CE2	2.56	0.41
1:E:481:TYR:O	1:E:482:TYR:C	2.62	0.41
1:A:51:TYR:O	1:A:52:GLY:O	2.38	0.41
1:A:169:THR:CG2	1:A:171:GLU:HB2	2.51	0.41
1:B:477:ARG:CG	1:B:477:ARG:NH1	2.84	0.41
1:C:3:LEU:O	1:C:5:ARG:N	2.51	0.41
1:C:56:LEU:HD13	1:C:105:ILE:HG13	2.02	0.41
1:C:124:GLU:H	1:C:124:GLU:HG3	1.65	0.41
1:C:225:MET:HG2	1:C:324:ARG:HH21	1.85	0.41
1:D:30:LEU:CD2	1:D:188:ARG:HB3	2.50	0.41
1:D:173:ILE:O	1:D:177:ILE:HG13	2.20	0.41
1:E:115:ASP:HA	1:E:120:ARG:HH11	1.86	0.41
1:F:473:ALA:O	1:F:474:LYS:C	2.64	0.41
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.80	0.40
1:A:123:LEU:CD2	1:A:123:LEU:N	2.77	0.40
1:A:222:LEU:CB	1:A:286:ILE:HD13	2.51	0.40
1:B:152:ARG:HG3	1:B:153:GLN:N	2.36	0.40
1:D:434:ASP:OD2	1:D:457:ARG:NH2	2.54	0.40
1:E:135:HIS:CD2	1:E:135:HIS:H	2.39	0.40
1:E:189:SER:C	1:E:191:ASN:N	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:HIS:CD2	1:E:344:LYS:HB2	2.56	0.40
1:E:472:MET:HB2	1:E:478:ASP:HB3	2.02	0.40
1:F:36:LYS:N	2:F:495:PO4:O1	2.54	0.40
1:F:60:PRO:HG3	1:F:136:ARG:HD3	2.02	0.40
1:F:456:ARG:HH11	1:F:456:ARG:CG	2.34	0.40
1:A:107:ALA:HB3	1:A:112:ILE:HD13	2.02	0.40
1:A:207:VAL:HG13	1:A:469:ILE:HG23	2.03	0.40
1:B:273:LEU:HD12	1:B:273:LEU:HA	1.84	0.40
1:C:294:LEU:HD12	1:C:340:LEU:O	2.21	0.40
1:C:364:ILE:HG13	1:C:422:VAL:HG22	2.02	0.40
1:D:226:LEU:HD22	1:D:230:LEU:CD1	2.51	0.40
1:E:333:VAL:CG1	1:E:334:GLN:N	2.84	0.40
1:F:123:LEU:CD2	1:F:123:LEU:N	2.80	0.40
1:F:124:GLU:HA	1:F:153:GLN:O	2.21	0.40
1:A:124:GLU:O	1:A:155:LYS:HG3	2.22	0.40
1:B:211:LEU:HB2	1:B:474:LYS:HZ2	1.87	0.40
1:C:23:GLU:OE2	1:C:51:TYR:OH	2.39	0.40
1:C:37:THR:O	1:C:40:ALA:HB3	2.21	0.40
1:C:169:THR:HG22	1:C:171:GLU:N	2.35	0.40
1:C:171:GLU:HG2	1:D:247:PRO:HG3	2.03	0.40
1:C:202:ILE:HG21	1:C:204:PHE:CZ	2.57	0.40
1:C:302:LYS:HB3	1:C:302:LYS:HE2	1.81	0.40
1:C:456:ARG:HH11	1:C:456:ARG:CG	2.32	0.40
1:F:190:GLU:HG3	1:F:199:VAL:HG11	2.04	0.40
1:F:208:ARG:CD	1:F:474:LYS:HG3	2.51	0.40
1:A:60:PRO:HB3	1:A:136:ARG:CZ	2.51	0.40
1:A:192:SER:C	1:A:194:ASP:N	2.79	0.40
1:B:280:LEU:HD12	1:B:280:LEU:HA	1.89	0.40
1:C:333:VAL:CG1	1:C:334:GLN:N	2.84	0.40
1:D:7:LEU:O	1:E:8:ILE:HA	2.21	0.40
1:D:202:ILE:HG21	1:D:204:PHE:CZ	2.57	0.40
1:D:261:GLU:OE1	1:D:264:LYS:HD2	2.21	0.40
1:A:135:HIS:CD2	1:A:135:HIS:H	2.38	0.40
1:A:251:VAL:HG23	1:A:252:LEU:N	2.36	0.40
1:A:355:GLN:NE2	1:A:358:ARG:NH2	2.68	0.40
1:A:405:GLN:HB3	1:A:406:ARG:H	1.70	0.40
1:B:294:LEU:HD12	1:B:340:LEU:O	2.21	0.40
1:B:476:THR:C	1:B:478:ASP:N	2.77	0.40
1:E:187:TYR:O	1:E:188:ARG:HD3	2.21	0.40
1:F:124:GLU:H	1:F:124:GLU:HG3	1.69	0.40
1:F:406:ARG:HA	1:F:406:ARG:NH1	2.30	0.40

All (1) 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)
1:B:268:ASP:OD2	1:E:371:ARG:NH1[1_455]	2.08	0.12

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	475/494 (96%)	442 (93%)	28 (6%)	5 (1%)	11	36
1	B	473/494 (96%)	443 (94%)	26 (6%)	4 (1%)	16	44
1	C	471/494 (95%)	435 (92%)	29 (6%)	7 (2%)	8	28
1	D	463/494 (94%)	433 (94%)	26 (6%)	4 (1%)	14	41
1	E	471/494 (95%)	441 (94%)	27 (6%)	3 (1%)	21	51
1	F	471/494 (95%)	439 (93%)	29 (6%)	3 (1%)	21	51
All	All	2824/2964 (95%)	2633 (93%)	165 (6%)	26 (1%)	14	41

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	GLY
1	C	52	GLY
1	F	52	GLY
1	A	52	GLY
1	A	484	SER
1	B	405	GLN
1	C	4	ARG
1	D	52	GLY
1	E	52	GLY
1	A	141	TYR
1	A	394	GLN
1	B	141	TYR

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Mol	Chain	Res	Type
1	C	141	TYR
1	D	141	TYR
1	E	419	GLU
1	F	141	TYR
1	B	165	SER
1	C	165	SER
1	C	419	GLU
1	D	165	SER
1	D	419	GLU
1	F	448	PRO
1	C	110	GLN
1	C	448	PRO
1	E	448	PRO
1	A	448	PRO

5.3.2 Protein sidechains [i](#)

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	413/427 (97%)	364 (88%)	49 (12%)	5	16
1	B	412/427 (96%)	367 (89%)	45 (11%)	6	20
1	C	411/427 (96%)	362 (88%)	49 (12%)	5	16
1	D	406/427 (95%)	361 (89%)	45 (11%)	6	20
1	E	411/427 (96%)	363 (88%)	48 (12%)	5	17
1	F	411/427 (96%)	365 (89%)	46 (11%)	6	19
All	All	2464/2562 (96%)	2182 (89%)	282 (11%)	5	18

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	22	LYS
1	A	87	THR
1	A	105	ILE

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Mol	Chain	Res	Type
1	A	110	GLN
1	A	112	ILE
1	A	123	LEU
1	A	124	GLU
1	A	140	ASN
1	A	158	LEU
1	A	169	THR
1	A	176	VAL
1	A	188	ARG
1	A	199	VAL
1	A	207	VAL
1	A	226	LEU
1	A	239	LEU
1	A	252	LEU
1	A	253	ARG
1	A	266	ASN
1	A	280	LEU
1	A	291	THR
1	A	309	LYS
1	A	314	LYS
1	A	318	GLU
1	A	324	ARG
1	A	336	LYS
1	A	353	ARG
1	A	354	GLU
1	A	355	GLN
1	A	357	GLN
1	A	364	ILE
1	A	370	TYR
1	A	394	GLN
1	A	411	ILE
1	A	419	GLU
1	A	430	GLU
1	A	438	VAL
1	A	440	LEU
1	A	441	VAL
1	A	442	VAL
1	A	448	PRO
1	A	455	GLN
1	A	457	ARG
1	A	468	VAL
1	A	472	MET

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Mol	Chain	Res	Type
1	A	474	LYS
1	A	476	THR
1	A	486	ARG
1	B	3	LEU
1	B	11	ARG
1	B	87	THR
1	B	105	ILE
1	B	110	GLN
1	B	111	THR
1	B	112	ILE
1	B	123	LEU
1	B	124	GLU
1	B	140	ASN
1	B	158	LEU
1	B	176	VAL
1	B	188	ARG
1	B	199	VAL
1	B	207	VAL
1	B	226	LEU
1	B	239	LEU
1	B	252	LEU
1	B	253	ARG
1	B	266	ASN
1	B	280	LEU
1	B	291	THR
1	B	309	LYS
1	B	314	LYS
1	B	318	GLU
1	B	324	ARG
1	B	336	LYS
1	B	353	ARG
1	B	354	GLU
1	B	355	GLN
1	B	357	GLN
1	B	364	ILE
1	B	370	TYR
1	B	391	PHE
1	B	392	VAL
1	B	411	ILE
1	B	419	GLU
1	B	430	GLU
1	B	438	VAL

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Mol	Chain	Res	Type
1	B	440	LEU
1	B	441	VAL
1	B	442	VAL
1	B	457	ARG
1	B	468	VAL
1	B	486	ARG
1	C	7	LEU
1	C	8	ILE
1	C	11	ARG
1	C	18	TYR
1	C	62	LYS
1	C	87	THR
1	C	105	ILE
1	C	110	GLN
1	C	112	ILE
1	C	123	LEU
1	C	124	GLU
1	C	127	SER
1	C	140	ASN
1	C	158	LEU
1	C	169	THR
1	C	176	VAL
1	C	188	ARG
1	C	199	VAL
1	C	226	LEU
1	C	239	LEU
1	C	252	LEU
1	C	253	ARG
1	C	266	ASN
1	C	280	LEU
1	C	291	THR
1	C	309	LYS
1	C	314	LYS
1	C	318	GLU
1	C	324	ARG
1	C	336	LYS
1	C	353	ARG
1	C	354	GLU
1	C	355	GLN
1	C	357	GLN
1	C	364	ILE
1	C	370	TYR

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Mol	Chain	Res	Type
1	C	391	PHE
1	C	406	ARG
1	C	411	ILE
1	C	419	GLU
1	C	430	GLU
1	C	438	VAL
1	C	440	LEU
1	C	441	VAL
1	C	442	VAL
1	C	448	PRO
1	C	457	ARG
1	C	468	VAL
1	C	486	ARG
1	D	1	MET
1	D	11	ARG
1	D	87	THR
1	D	105	ILE
1	D	110	GLN
1	D	111	THR
1	D	112	ILE
1	D	123	LEU
1	D	124	GLU
1	D	140	ASN
1	D	158	LEU
1	D	169	THR
1	D	176	VAL
1	D	188	ARG
1	D	199	VAL
1	D	207	VAL
1	D	226	LEU
1	D	239	LEU
1	D	252	LEU
1	D	253	ARG
1	D	266	ASN
1	D	280	LEU
1	D	291	THR
1	D	309	LYS
1	D	314	LYS
1	D	318	GLU
1	D	324	ARG
1	D	336	LYS
1	D	353	ARG

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Mol	Chain	Res	Type
1	D	354	GLU
1	D	355	GLN
1	D	357	GLN
1	D	364	ILE
1	D	370	TYR
1	D	411	ILE
1	D	419	GLU
1	D	430	GLU
1	D	438	VAL
1	D	440	LEU
1	D	441	VAL
1	D	442	VAL
1	D	457	ARG
1	D	468	VAL
1	D	474	LYS
1	D	477	ARG
1	E	11	ARG
1	E	87	THR
1	E	105	ILE
1	E	110	GLN
1	E	112	ILE
1	E	123	LEU
1	E	124	GLU
1	E	140	ASN
1	E	158	LEU
1	E	169	THR
1	E	176	VAL
1	E	188	ARG
1	E	199	VAL
1	E	207	VAL
1	E	226	LEU
1	E	239	LEU
1	E	252	LEU
1	E	253	ARG
1	E	266	ASN
1	E	280	LEU
1	E	291	THR
1	E	309	LYS
1	E	314	LYS
1	E	318	GLU
1	E	324	ARG
1	E	336	LYS

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Mol	Chain	Res	Type
1	E	353	ARG
1	E	354	GLU
1	E	355	GLN
1	E	357	GLN
1	E	363	LYS
1	E	364	ILE
1	E	370	TYR
1	E	406	ARG
1	E	407	GLU
1	E	411	ILE
1	E	419	GLU
1	E	430	GLU
1	E	438	VAL
1	E	440	LEU
1	E	441	VAL
1	E	442	VAL
1	E	457	ARG
1	E	468	VAL
1	E	474	LYS
1	E	477	ARG
1	E	486	ARG
1	E	487	GLN
1	F	2	VAL
1	F	5	ARG
1	F	11	ARG
1	F	87	THR
1	F	105	ILE
1	F	110	GLN
1	F	112	ILE
1	F	123	LEU
1	F	124	GLU
1	F	140	ASN
1	F	158	LEU
1	F	169	THR
1	F	176	VAL
1	F	188	ARG
1	F	199	VAL
1	F	207	VAL
1	F	226	LEU
1	F	239	LEU
1	F	252	LEU
1	F	253	ARG

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Mol	Chain	Res	Type
1	F	266	ASN
1	F	280	LEU
1	F	291	THR
1	F	309	LYS
1	F	314	LYS
1	F	318	GLU
1	F	324	ARG
1	F	336	LYS
1	F	353	ARG
1	F	354	GLU
1	F	355	GLN
1	F	357	GLN
1	F	364	ILE
1	F	392	VAL
1	F	411	ILE
1	F	419	GLU
1	F	430	GLU
1	F	438	VAL
1	F	440	LEU
1	F	441	VAL
1	F	445	GLU
1	F	448	PRO
1	F	455	GLN
1	F	457	ARG
1	F	468	VAL
1	F	474	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	25	ASN
1	A	110	GLN
1	A	135	HIS
1	A	140	ASN
1	A	153	GLN
1	A	179	ASN
1	A	184	HIS
1	A	259	ASN
1	A	266	ASN
1	A	292	GLN
1	A	342	HIS

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Mol	Chain	Res	Type
1	A	355	GLN
1	A	360	GLN
1	A	369	ASN
1	A	463	HIS
1	B	9	GLN
1	B	14	GLN
1	B	25	ASN
1	B	110	GLN
1	B	135	HIS
1	B	140	ASN
1	B	153	GLN
1	B	179	ASN
1	B	184	HIS
1	B	259	ASN
1	B	266	ASN
1	B	292	GLN
1	B	342	HIS
1	B	360	GLN
1	B	405	GLN
1	B	463	HIS
1	C	14	GLN
1	C	25	ASN
1	C	110	GLN
1	C	135	HIS
1	C	140	ASN
1	C	153	GLN
1	C	179	ASN
1	C	184	HIS
1	C	259	ASN
1	C	266	ASN
1	C	283	HIS
1	C	292	GLN
1	C	342	HIS
1	C	355	GLN
1	C	360	GLN
1	C	408	GLN
1	C	463	HIS
1	D	9	GLN
1	D	14	GLN
1	D	25	ASN
1	D	110	GLN
1	D	135	HIS

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Mol	Chain	Res	Type
1	D	140	ASN
1	D	153	GLN
1	D	156	ASN
1	D	179	ASN
1	D	184	HIS
1	D	259	ASN
1	D	266	ASN
1	D	292	GLN
1	D	342	HIS
1	D	360	GLN
1	D	369	ASN
1	D	463	HIS
1	E	9	GLN
1	E	14	GLN
1	E	25	ASN
1	E	110	GLN
1	E	135	HIS
1	E	140	ASN
1	E	153	GLN
1	E	179	ASN
1	E	184	HIS
1	E	259	ASN
1	E	266	ASN
1	E	292	GLN
1	E	342	HIS
1	E	355	GLN
1	E	360	GLN
1	E	408	GLN
1	E	421	ASN
1	E	463	HIS
1	F	14	GLN
1	F	25	ASN
1	F	110	GLN
1	F	135	HIS
1	F	140	ASN
1	F	153	GLN
1	F	179	ASN
1	F	184	HIS
1	F	259	ASN
1	F	266	ASN
1	F	283	HIS
1	F	292	GLN

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Mol	Chain	Res	Type
1	F	342	HIS
1	F	355	GLN
1	F	360	GLN
1	F	369	ASN
1	F	408	GLN
1	F	463	HIS
1	F	487	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	D	495	-	4,4,4	1.67	0	6,6,6	0.44	0
2	PO4	E	495	-	4,4,4	1.71	0	6,6,6	0.46	0
2	PO4	C	495	-	4,4,4	1.74	1 (25%)	6,6,6	0.50	0
2	PO4	B	495	-	4,4,4	1.72	1 (25%)	6,6,6	0.46	0
2	PO4	A	495	-	4,4,4	1.91	3 (75%)	6,6,6	0.44	0
2	PO4	F	495	-	4,4,4	1.66	0	6,6,6	0.45	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	495	PO4	P-O4	-2.26	1.48	1.54
2	C	495	PO4	P-O3	-2.24	1.48	1.54
2	A	495	PO4	P-O3	-2.14	1.48	1.54
2	A	495	PO4	P-O2	-2.13	1.48	1.54
2	B	495	PO4	P-O4	-2.05	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	495	PO4	1	0
2	C	495	PO4	2	0
2	B	495	PO4	1	0
2	A	495	PO4	5	0
2	F	495	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	479/494 (96%)	0.13	19 (3%)	42 34	24, 55, 97, 109	0
1	B	477/494 (96%)	0.03	13 (2%)	56 47	24, 57, 95, 117	0
1	C	475/494 (96%)	0.19	18 (3%)	44 36	30, 62, 99, 119	0
1	D	469/494 (94%)	0.18	17 (3%)	46 38	30, 67, 100, 116	0
1	E	475/494 (96%)	0.05	7 (1%)	72 64	25, 58, 99, 118	0
1	F	475/494 (96%)	0.17	7 (1%)	72 64	35, 65, 102, 126	0
All	All	2850/2964 (96%)	0.13	81 (2%)	55 46	24, 61, 99, 126	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	269	LEU	6.4
1	C	120	ARG	4.4
1	D	461	GLY	4.2
1	B	269	LEU	4.0
1	C	262	MET	3.5
1	F	97	LYS	3.5
1	B	263	ALA	3.4
1	C	266	ASN	3.4
1	C	270	ARG	3.3
1	E	263	ALA	3.2
1	B	166	PRO	3.1
1	D	335	ALA	3.0
1	E	308	ALA	3.0
1	D	308	ALA	3.0
1	F	166	PRO	3.0
1	D	269	LEU	2.9
1	D	53	GLY	2.9
1	D	164	ALA	2.9
1	C	121	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	265	GLY	2.9
1	E	264	LYS	2.9
1	B	460	THR	2.8
1	B	317	LYS	2.8
1	C	416	ALA	2.8
1	A	269	LEU	2.8
1	A	405	GLN	2.8
1	B	268	ASP	2.7
1	B	333	VAL	2.7
1	A	309	LYS	2.7
1	D	307	GLU	2.6
1	C	311	GLY	2.6
1	B	385	GLY	2.5
1	D	166	PRO	2.5
1	C	202	ILE	2.5
1	E	371	ARG	2.5
1	F	202	ILE	2.4
1	B	52	GLY	2.4
1	B	392	VAL	2.4
1	A	385	GLY	2.4
1	F	429	GLY	2.4
1	A	62	LYS	2.4
1	C	98	ALA	2.4
1	D	310	ALA	2.4
1	D	265	GLY	2.4
1	A	155	LYS	2.4
1	F	392	VAL	2.4
1	C	427	SER	2.3
1	B	410	LEU	2.3
1	C	166	PRO	2.3
1	B	165	SER	2.3
1	C	312	SER	2.3
1	A	305	TYR	2.3
1	A	53	GLY	2.3
1	C	269	LEU	2.3
1	F	92	PRO	2.3
1	A	393	GLY	2.3
1	D	263	ALA	2.2
1	A	310	ALA	2.2
1	D	202	ILE	2.2
1	A	125	ASP	2.2
1	C	119	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	53	GLY	2.2
1	A	306	GLU	2.2
1	A	267	HIS	2.1
1	E	267	HIS	2.1
1	A	311	GLY	2.1
1	F	269	LEU	2.1
1	A	206	TRP	2.1
1	D	328	ALA	2.1
1	A	265	GLY	2.1
1	A	121	ILE	2.1
1	A	202	ILE	2.1
1	C	267	HIS	2.1
1	E	201	GLY	2.1
1	C	263	ALA	2.1
1	D	52	GLY	2.0
1	D	239	LEU	2.0
1	D	410	LEU	2.0
1	A	201	GLY	2.0
1	C	88	GLY	2.0
1	D	460	THR	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	F	495	5/5	0.76	0.16	118,118,119,119	0
2	PO4	D	495	5/5	0.79	0.17	124,125,125,126	0
2	PO4	C	495	5/5	0.82	0.17	84,86,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	E	495	5/5	0.83	0.20	111,112,112,113	0
2	PO4	A	495	5/5	0.86	0.17	97,98,98,99	0
2	PO4	B	495	5/5	0.88	0.21	105,105,106,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.