



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:49 PM EDT

PDB ID : 3E1Y / pdb_00003e1y
Title : Crystal structure of human eRF1/eRF3 complex
Authors : Cheng, Z.; Lim, M.; Kong, C.; Song, H.
Deposited on : 2008-08-05
Resolution : 3.80 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

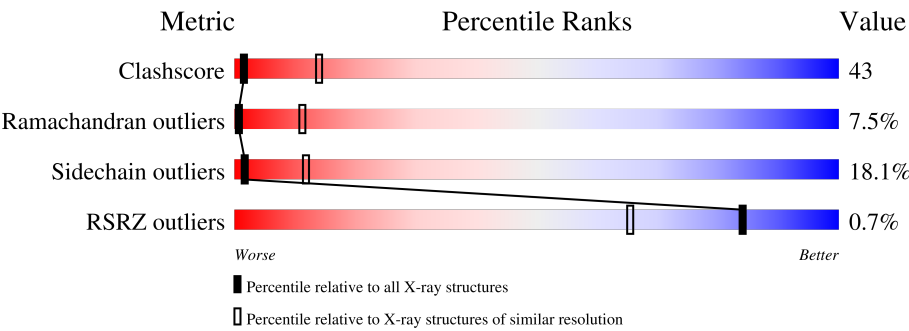
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	451	33%37%13%•16%
1	B	451	% 33%36%14%•16%
1	C	451	% 35%29%6%•29%
1	D	451	% 35%29%5%•29%
2	E	204	26%45%17%8%•
2	F	204	27%44%17%8%•
2	G	204	% 31%41%20%••

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Mol	Chain	Length	Quality of chain
2	H	204	30% 43% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17110 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 Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2987	1908	511	558	10			
1	B	380	Total	C	N	O	S	0	0	0
			2987	1908	511	558	10			
1	C	318	Total	C	N	O	S	0	0	0
			2511	1617	414	470	10			
1	D	318	Total	C	N	O	S	0	0	0
			2511	1617	414	470	10			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP P62495
A	-12	ARG	-	expression tag	UNP P62495
A	-11	GLY	-	expression tag	UNP P62495
A	-10	SER	-	expression tag	UNP P62495
A	-9	HIS	-	expression tag	UNP P62495
A	-8	HIS	-	expression tag	UNP P62495
A	-7	HIS	-	expression tag	UNP P62495
A	-6	HIS	-	expression tag	UNP P62495
A	-5	HIS	-	expression tag	UNP P62495
A	-4	HIS	-	expression tag	UNP P62495
A	-3	GLY	-	expression tag	UNP P62495
A	-2	MET	-	expression tag	UNP P62495
A	-1	ALA	-	expression tag	UNP P62495
A	0	SER	-	expression tag	UNP P62495
B	-13	MET	-	expression tag	UNP P62495
B	-12	ARG	-	expression tag	UNP P62495
B	-11	GLY	-	expression tag	UNP P62495
B	-10	SER	-	expression tag	UNP P62495
B	-9	HIS	-	expression tag	UNP P62495
B	-8	HIS	-	expression tag	UNP P62495
B	-7	HIS	-	expression tag	UNP P62495

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP P62495
B	-5	HIS	-	expression tag	UNP P62495
B	-4	HIS	-	expression tag	UNP P62495
B	-3	GLY	-	expression tag	UNP P62495
B	-2	MET	-	expression tag	UNP P62495
B	-1	ALA	-	expression tag	UNP P62495
B	0	SER	-	expression tag	UNP P62495
C	-13	MET	-	expression tag	UNP P62495
C	-12	ARG	-	expression tag	UNP P62495
C	-11	GLY	-	expression tag	UNP P62495
C	-10	SER	-	expression tag	UNP P62495
C	-9	HIS	-	expression tag	UNP P62495
C	-8	HIS	-	expression tag	UNP P62495
C	-7	HIS	-	expression tag	UNP P62495
C	-6	HIS	-	expression tag	UNP P62495
C	-5	HIS	-	expression tag	UNP P62495
C	-4	HIS	-	expression tag	UNP P62495
C	-3	GLY	-	expression tag	UNP P62495
C	-2	MET	-	expression tag	UNP P62495
C	-1	ALA	-	expression tag	UNP P62495
C	0	SER	-	expression tag	UNP P62495
D	-13	MET	-	expression tag	UNP P62495
D	-12	ARG	-	expression tag	UNP P62495
D	-11	GLY	-	expression tag	UNP P62495
D	-10	SER	-	expression tag	UNP P62495
D	-9	HIS	-	expression tag	UNP P62495
D	-8	HIS	-	expression tag	UNP P62495
D	-7	HIS	-	expression tag	UNP P62495
D	-6	HIS	-	expression tag	UNP P62495
D	-5	HIS	-	expression tag	UNP P62495
D	-4	HIS	-	expression tag	UNP P62495
D	-3	GLY	-	expression tag	UNP P62495
D	-2	MET	-	expression tag	UNP P62495
D	-1	ALA	-	expression tag	UNP P62495
D	0	SER	-	expression tag	UNP P62495

- Molecule 2 is a protein called Eukaryotic peptide chain release factor GTP-binding subunit ERF3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	195	Total	C	N	O	S	0	0	0
			1513	960	261	280	12			

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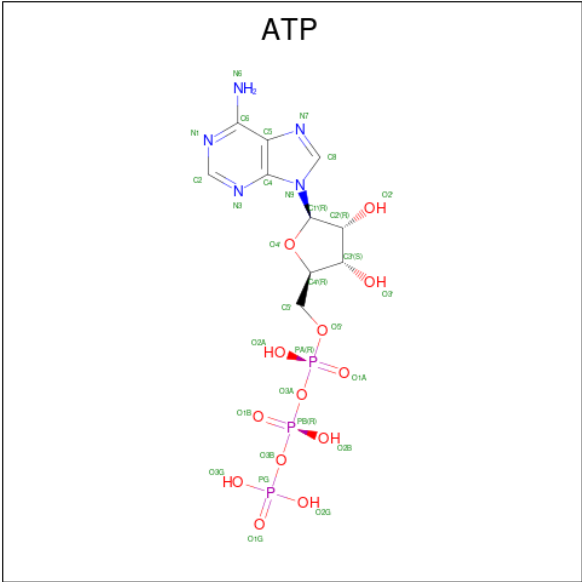
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	195	Total	C	N	O	S	0	0	0
			1513	960	261	280	12			
2	G	195	Total	C	N	O	S	0	0	0
			1513	960	261	280	12			
2	H	195	Total	C	N	O	S	0	0	0
			1513	960	261	280	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	434	GLY	-	expression tag	UNP P15170
E	435	PRO	-	expression tag	UNP P15170
E	436	LEU	-	expression tag	UNP P15170
E	437	GLY	-	expression tag	UNP P15170
E	438	SER	-	expression tag	UNP P15170
F	434	GLY	-	expression tag	UNP P15170
F	435	PRO	-	expression tag	UNP P15170
F	436	LEU	-	expression tag	UNP P15170
F	437	GLY	-	expression tag	UNP P15170
F	438	SER	-	expression tag	UNP P15170
G	434	GLY	-	expression tag	UNP P15170
G	435	PRO	-	expression tag	UNP P15170
G	436	LEU	-	expression tag	UNP P15170
G	437	GLY	-	expression tag	UNP P15170
G	438	SER	-	expression tag	UNP P15170
H	434	GLY	-	expression tag	UNP P15170
H	435	PRO	-	expression tag	UNP P15170
H	436	LEU	-	expression tag	UNP P15170
H	437	GLY	-	expression tag	UNP P15170
H	438	SER	-	expression tag	UNP P15170

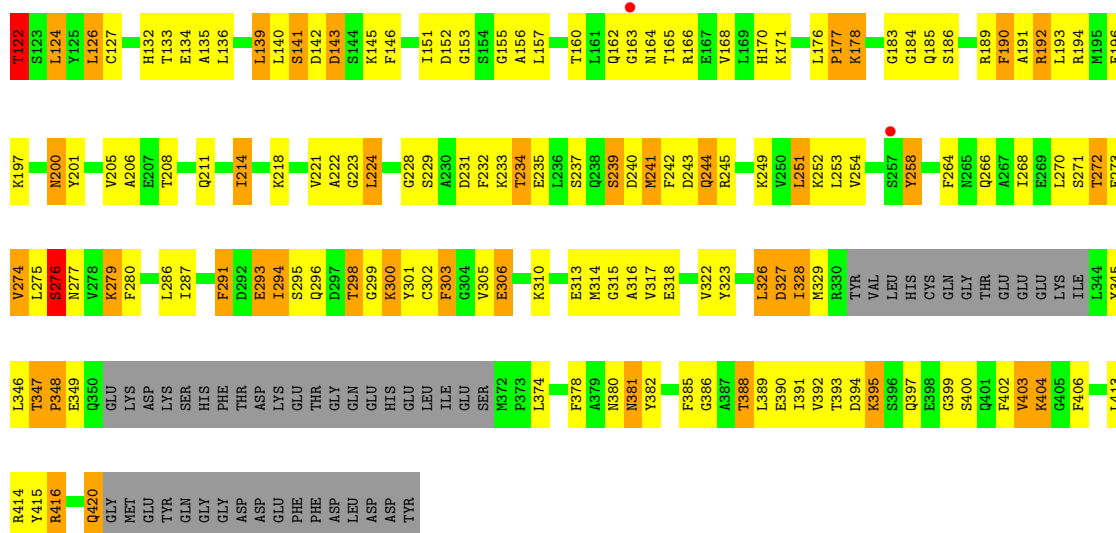
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



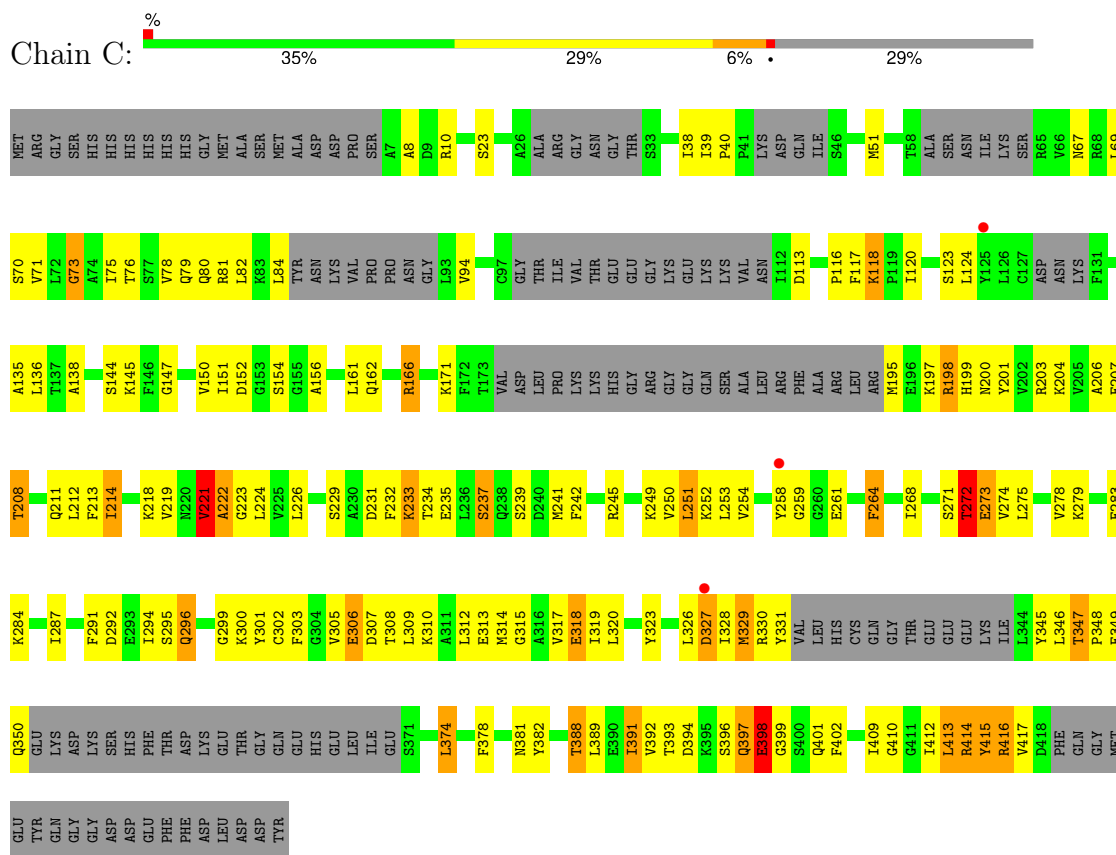
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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.

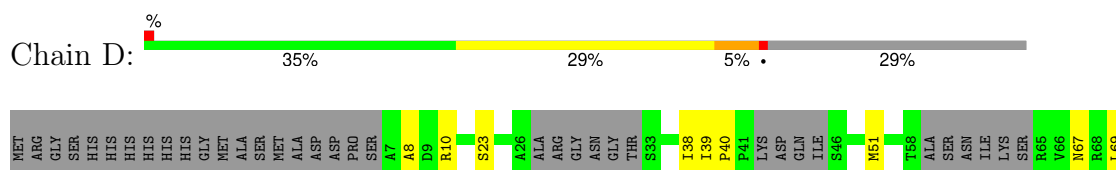
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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| S60 | S61 | T62 | K63 | S64 | R65 | V66 | H67 | R68 | L69 | S70 | V71 | L72 | G73 | A74 | S77 | V78 | Q79 | S80 | R81 | L82 | K83 | L84 | S85 | R86 | K87 | V88 | P89 | N90 | P91 | G92 | L93 | V94 | P95 | V96 | C97 | I100 | T101 | T102 | E103 | E104 | G105 | K106 | K108 | K109 | V110 | M111 | I112 | D113 | F114 | E115 | P116 | F117 | K118 | P119 | I120 |
| MET | ARG | GLY | SER | HIS | HIS | HIS | HIS | HIS | HIS | GLY | MET | ALA | SER | MET | SER | ASP | PRO | SER | A7 | R10 | E13 | I14 | I17 | K18 | K19 | L20 | I21 | K22 | S23 | L24 | E25 | A26 | A27 | R28 | G31 | I35 | I38 | I39 | P40 | K42 | D43 | Q44 | I45 | S46 | R47 | M51 | L52 | T58 | A59 | | | | | | |

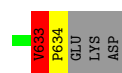


• Molecule 1: Eukaryotic peptide chain release factor subunit 1

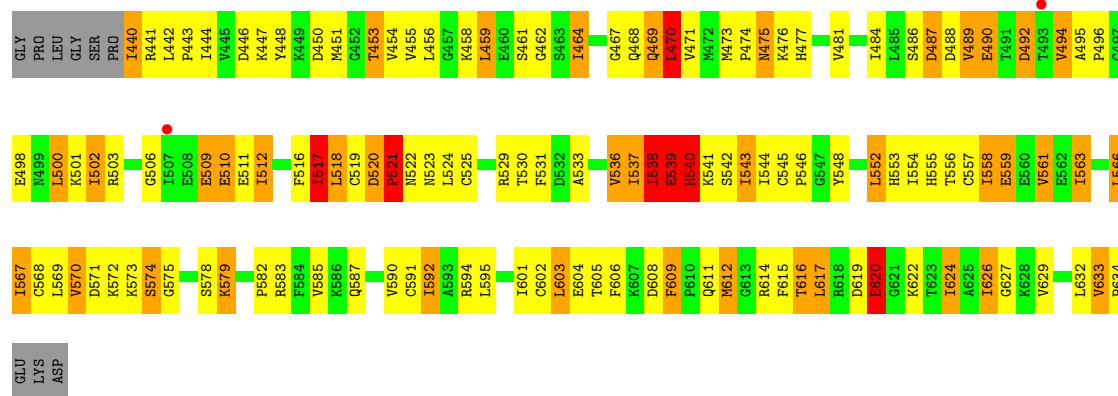


• Molecule 1: Eukaryotic peptide chain release factor subunit 1

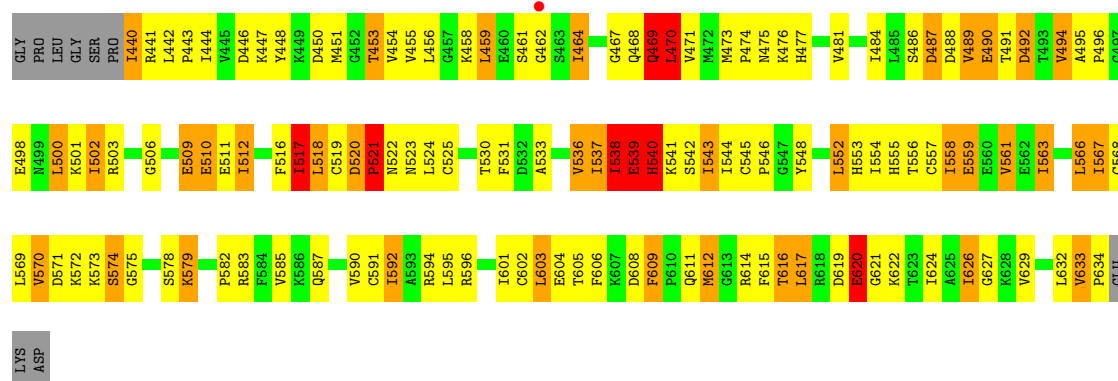




• Molecule 2: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A



• Molecule 2: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	173.97Å 173.97Å 119.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 30.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.80) 99.9 (30.00-3.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.260 , 0.304 0.279 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	151.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 271.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.430 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17110	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: ATP

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	0.65	2/3033 (0.1%)	0.96	9/4077 (0.2%)
1	B	0.64	1/3033 (0.0%)	1.00	10/4077 (0.2%)
1	C	0.45	0/2544	0.86	3/3413 (0.1%)
1	D	0.45	0/2544	0.86	2/3413 (0.1%)
2	E	0.69	0/1534	1.28	23/2068 (1.1%)
2	F	0.71	1/1534 (0.1%)	1.26	19/2068 (0.9%)
2	G	0.63	0/1534	1.14	15/2068 (0.7%)
2	H	0.64	0/1534	1.15	16/2068 (0.8%)
All	All	0.60	4/17290 (0.0%)	1.04	97/23252 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	E	0	10
2	F	0	10
2	G	0	5
2	H	0	5
All	All	0	31

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	ARG	CD-NE	8.04	1.57	1.46
2	F	524	LEU	N-CA	6.44	1.50	1.46
1	A	416	ARG	CZ-NH2	-5.70	1.26	1.33
1	B	416	ARG	NE-CZ	5.46	1.39	1.33

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	539	GLU	N-CA-C	-16.96	82.38	108.67
2	H	539	GLU	N-CA-C	-16.36	83.31	108.67
2	E	539	GLU	N-CA-C	-14.02	84.12	108.23
1	B	299	GLY	N-CA-C	-10.39	88.55	113.18
2	F	537	ILE	N-CA-C	-10.36	91.14	106.88
2	E	470	LEU	N-CA-C	10.10	124.49	109.95
2	F	470	LEU	N-CA-C	9.87	124.17	109.95
2	E	537	ILE	N-CA-C	-9.63	90.82	106.32
2	F	540	HIS	N-CA-C	9.35	130.71	110.80
1	B	415	TYR	N-CA-C	9.15	119.99	108.19
2	E	540	HIS	N-CA-C	8.59	129.10	110.80
2	H	518	LEU	N-CA-C	8.32	128.53	110.80
2	G	518	LEU	N-CA-C	7.96	127.77	110.80
2	H	609	PHE	CA-C-N	7.81	127.45	119.56
2	H	609	PHE	C-N-CA	7.81	127.45	119.56
2	E	518	LEU	N-CA-C	7.73	127.26	110.80
2	G	540	HIS	N-CA-C	7.71	127.23	110.80
2	F	518	LEU	N-CA-C	7.62	127.03	110.80
2	G	609	PHE	CA-C-N	7.49	127.20	119.56
2	G	609	PHE	C-N-CA	7.49	127.20	119.56
2	H	540	HIS	N-CA-C	7.46	126.68	110.80
1	B	293	GLU	N-CA-C	-7.14	101.75	112.04
2	F	633	VAL	N-CA-C	6.99	115.08	107.60
1	A	293	GLU	N-CA-C	-6.95	102.04	112.04
2	H	470	LEU	N-CA-CB	6.79	121.97	110.49
2	F	529	ARG	N-CA-C	6.79	122.39	113.30
2	E	633	VAL	N-CA-C	6.69	114.76	107.60
2	E	536	VAL	N-CA-C	6.55	122.97	109.34
2	F	536	VAL	N-CA-C	6.50	122.85	109.34
1	B	298	THR	N-CA-C	6.46	124.56	110.80
2	F	442	LEU	CA-C-N	6.30	127.29	119.98
2	F	442	LEU	C-N-CA	6.30	127.29	119.98
2	G	470	LEU	N-CA-CB	6.28	121.11	110.49
2	G	509	GLU	N-CA-C	6.21	121.02	113.38
2	H	517	ILE	CB-CA-C	6.20	118.60	110.91
2	H	509	GLU	N-CA-C	6.15	120.95	113.38
2	G	517	ILE	CB-CA-C	6.15	118.53	110.91
2	H	517	ILE	N-CA-C	-6.12	99.77	108.58
2	G	517	ILE	N-CA-C	-6.07	99.85	108.58
2	E	475	ASN	CB-CA-C	-6.00	101.13	110.37
1	C	264	PHE	N-CA-C	-5.98	105.07	112.90
2	E	442	LEU	CA-C-N	5.93	126.86	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	442	LEU	C-N-CA	5.93	126.86	119.98
2	F	620	GLU	CB-CA-C	-5.92	109.18	117.23
2	G	620	GLU	CB-CA-C	-5.89	109.22	117.23
2	G	492	ASP	N-CA-C	-5.87	107.93	114.62
1	B	143	ASP	N-CA-C	5.87	119.51	110.42
2	H	620	GLU	CB-CA-C	-5.85	109.27	117.23
2	E	620	GLU	CB-CA-C	-5.84	109.28	117.23
1	A	143	ASP	N-CA-C	5.84	119.47	110.42
2	H	492	ASP	N-CA-C	-5.83	107.98	114.62
2	E	626	ILE	N-CA-C	5.67	116.03	107.75
2	F	626	ILE	N-CA-C	5.67	116.02	107.75
2	H	603	LEU	N-CA-C	5.63	117.35	108.96
2	G	603	LEU	N-CA-C	5.62	117.34	108.96
2	F	525	CYS	N-CA-CB	5.62	119.59	110.32
1	A	234	THR	N-CA-C	-5.61	106.28	113.01
2	H	538	ILE	N-CA-C	-5.60	97.69	109.34
2	E	524	LEU	N-CA-C	5.55	113.33	108.78
1	B	234	THR	N-CA-C	-5.47	106.45	113.01
2	H	517	ILE	O-C-N	-5.46	116.73	122.95
1	A	89	PRO	CA-C-N	5.42	126.61	119.84
1	A	89	PRO	C-N-CA	5.42	126.61	119.84
2	F	446	ASP	N-CA-C	5.41	117.61	109.23
1	D	264	PHE	N-CA-C	-5.40	105.42	112.23
2	F	507	ILE	N-CA-C	5.40	116.05	110.82
2	E	446	ASP	N-CA-C	5.36	117.54	109.23
1	C	295	SER	N-CA-C	-5.36	105.98	113.37
2	G	538	ILE	N-CA-C	-5.33	98.25	109.34
1	D	295	SER	N-CA-C	-5.33	106.02	113.37
2	E	521	PRO	N-CA-C	5.28	123.34	112.47
1	B	71	VAL	CB-CA-C	-5.28	105.13	111.88
2	E	517	ILE	CB-CA-C	5.27	118.00	111.15
2	E	524	LEU	CA-C-O	5.25	120.99	117.94
2	H	561	VAL	N-CA-C	5.24	115.26	108.35
2	E	521	PRO	CA-C-N	5.23	131.12	121.70
2	E	521	PRO	C-N-CA	5.23	131.12	121.70
2	G	517	ILE	O-C-N	-5.22	117.00	122.95
2	E	583	ARG	N-CA-C	-5.21	105.29	111.69
2	G	561	VAL	N-CA-C	5.20	115.22	108.35
2	F	583	ARG	N-CA-C	-5.20	105.30	111.69
1	A	295	SER	N-CA-C	-5.16	107.05	113.19
2	E	540	HIS	N-CA-CB	-5.16	101.77	110.49
1	A	300	LYS	N-CA-C	-5.16	104.48	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	464	ILE	N-CA-C	5.15	115.27	107.75
2	F	521	PRO	CA-C-N	5.14	130.96	121.70
2	F	521	PRO	C-N-CA	5.14	130.96	121.70
2	H	469	GLN	O-C-N	-5.13	117.47	123.27
1	C	296	GLN	N-CA-C	5.09	117.75	109.24
2	E	507	ILE	N-CA-C	5.09	115.76	110.82
1	A	88	VAL	CA-C-N	5.09	125.62	120.38
1	A	88	VAL	C-N-CA	5.09	125.62	120.38
2	F	517	ILE	CB-CA-C	5.09	117.77	111.15
2	E	464	ILE	N-CA-C	5.06	115.14	107.75
1	B	89	PRO	CA-C-N	5.03	126.13	119.84
1	B	89	PRO	C-N-CA	5.03	126.13	119.84
1	B	295	SER	N-CA-C	-5.01	106.99	113.01

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	298	THR	Peptide
2	E	469	GLN	Peptide
2	E	473	MET	Peptide
2	E	517	ILE	Peptide
2	E	521	PRO	Peptide
2	E	528	GLY	Peptide
2	E	536	VAL	Peptide
2	E	538	ILE	Peptide
2	E	539	GLU	Peptide
2	E	543	ILE	Peptide
2	E	544	ILE	Peptide
2	F	469	GLN	Peptide
2	F	473	MET	Peptide
2	F	517	ILE	Peptide
2	F	521	PRO	Peptide
2	F	524	LEU	Peptide
2	F	528	GLY	Peptide
2	F	536	VAL	Peptide
2	F	539	GLU	Peptide
2	F	543	ILE	Peptide
2	F	544	ILE	Peptide
2	G	469	GLN	Peptide
2	G	517	ILE	Peptide
2	G	521	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	G	538	ILE	Peptide
2	G	539	GLU	Peptide
2	H	469	GLN	Peptide
2	H	517	ILE	Peptide
2	H	521	PRO	Peptide
2	H	538	ILE	Peptide
2	H	539	GLU	Peptide

5.2 Too-close contacts [i](#)

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	2987	0	3054	241	0
1	B	2987	0	3054	235	0
1	C	2511	0	2552	130	0
1	D	2511	0	2552	129	0
2	E	1513	0	1582	184	0
2	F	1513	0	1582	186	0
2	G	1513	0	1582	194	0
2	H	1513	0	1582	192	0
3	A	31	0	12	3	0
3	B	31	0	12	0	0
All	All	17110	0	17564	1478	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 43.

All (1478) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:541:LYS:HG2	2:G:587:GLN:NE2	1.21	1.53
2:H:541:LYS:HG2	2:H:587:GLN:NE2	1.20	1.45
2:E:541:LYS:HG2	2:E:587:GLN:NE2	1.27	1.41
2:F:541:LYS:HG2	2:F:587:GLN:NE2	1.30	1.38
2:F:540:HIS:HB3	2:F:541:LYS:CA	1.50	1.37
2:H:540:HIS:HB3	2:H:541:LYS:CA	1.52	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:540:HIS:HB3	2:G:541:LYS:CA	1.52	1.37
1:C:252:LYS:HE2	1:C:274:VAL:CG2	1.56	1.35
2:E:540:HIS:HB3	2:E:541:LYS:CA	1.50	1.34
1:D:252:LYS:HE2	1:D:274:VAL:CG2	1.56	1.34
2:E:540:HIS:CB	2:E:541:LYS:HA	1.51	1.33
1:B:118:LYS:CD	1:B:119:PRO:HD3	1.57	1.33
2:G:540:HIS:CB	2:G:541:LYS:HA	1.56	1.32
1:A:118:LYS:CD	1:A:119:PRO:HD3	1.58	1.31
1:A:118:LYS:CE	1:A:119:PRO:HD3	1.61	1.30
1:A:91:ASN:O	1:A:120:ILE:HG22	1.16	1.28
2:G:541:LYS:HG2	2:G:587:GLN:CD	1.59	1.27
2:E:541:LYS:HG2	2:E:587:GLN:CD	1.59	1.27
1:B:118:LYS:CE	1:B:119:PRO:HD3	1.64	1.26
2:E:541:LYS:HB3	2:E:587:GLN:OE1	1.35	1.26
1:A:118:LYS:HE3	1:A:119:PRO:CD	1.65	1.25
2:F:540:HIS:CB	2:F:541:LYS:HA	1.51	1.25
2:H:633:VAL:HG12	2:H:634:PRO:CD	1.66	1.25
2:G:633:VAL:HG12	2:G:634:PRO:CD	1.66	1.25
2:H:541:LYS:HG2	2:H:587:GLN:CD	1.62	1.25
1:B:91:ASN:O	1:B:120:ILE:HG22	1.18	1.25
2:H:540:HIS:CB	2:H:541:LYS:HA	1.55	1.24
2:F:541:LYS:HG2	2:F:587:GLN:CD	1.62	1.23
2:G:541:LYS:HB3	2:G:587:GLN:OE1	1.33	1.23
2:F:541:LYS:HB3	2:F:587:GLN:OE1	1.36	1.23
1:B:118:LYS:HE3	1:B:119:PRO:CD	1.69	1.21
2:H:541:LYS:HB3	2:H:587:GLN:OE1	1.38	1.20
2:G:633:VAL:CG1	2:G:634:PRO:HD3	1.71	1.20
2:E:541:LYS:CG	2:E:587:GLN:NE2	2.05	1.19
2:H:633:VAL:CG1	2:H:634:PRO:HD3	1.71	1.19
1:D:252:LYS:HE2	1:D:274:VAL:HG21	1.19	1.18
2:H:545:CYS:HB2	2:H:546:PRO:HD2	1.20	1.16
1:C:347:THR:HB	1:C:348:PRO:HD2	1.28	1.15
2:H:541:LYS:CG	2:H:587:GLN:NE2	2.08	1.15
2:F:541:LYS:CG	2:F:587:GLN:NE2	2.09	1.15
2:G:541:LYS:CG	2:G:587:GLN:NE2	2.09	1.14
1:C:252:LYS:HE2	1:C:274:VAL:HG21	1.20	1.13
1:A:115:GLU:CG	1:A:116:PRO:HD2	1.78	1.12
2:G:545:CYS:HB2	2:G:546:PRO:HD2	1.19	1.12
2:H:541:LYS:CG	2:H:587:GLN:HE22	1.62	1.12
2:E:545:CYS:HB2	2:E:546:PRO:HD2	1.12	1.11
1:D:347:THR:HB	1:D:348:PRO:HD2	1.29	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLU:CG	1:B:116:PRO:HD2	1.78	1.11
2:G:541:LYS:CB	2:G:587:GLN:OE1	1.97	1.11
2:G:541:LYS:CG	2:G:587:GLN:HE22	1.64	1.10
2:F:545:CYS:HB2	2:F:546:PRO:HD2	1.14	1.09
2:F:473:MET:HE1	2:F:525:CYS:O	1.50	1.09
2:G:444:ILE:HG23	2:G:455:VAL:HG13	1.35	1.08
2:E:541:LYS:CD	2:E:587:GLN:HE22	1.64	1.08
2:E:541:LYS:CE	2:E:587:GLN:HE22	1.66	1.08
1:A:347:THR:HB	1:A:348:PRO:HD2	1.13	1.08
2:G:440:ILE:HB	2:G:462:GLY:HA3	1.08	1.08
2:H:440:ILE:HB	2:H:462:GLY:HA3	1.09	1.08
1:B:347:THR:HB	1:B:348:PRO:HD2	1.14	1.07
1:B:115:GLU:HG3	1:B:116:PRO:CD	1.83	1.07
1:B:115:GLU:HG3	1:B:116:PRO:HD2	1.35	1.07
2:F:473:MET:CE	2:F:525:CYS:O	2.03	1.06
1:D:287:ILE:HG21	1:D:398:GLU:O	1.53	1.06
2:H:444:ILE:HG23	2:H:455:VAL:HG13	1.37	1.06
2:H:541:LYS:CB	2:H:587:GLN:OE1	2.03	1.06
2:F:541:LYS:CE	2:F:587:GLN:HE22	1.69	1.06
1:A:115:GLU:HG3	1:A:116:PRO:CD	1.85	1.05
1:C:287:ILE:HG21	1:C:398:GLU:O	1.55	1.05
1:D:252:LYS:HE2	1:D:274:VAL:HG23	1.37	1.05
2:F:541:LYS:CD	2:F:587:GLN:HE22	1.68	1.05
1:D:312:LEU:HD12	1:D:317:VAL:HG21	1.36	1.04
1:D:391:ILE:HD12	1:D:391:ILE:H	1.23	1.04
2:E:541:LYS:CB	2:E:587:GLN:OE1	2.05	1.04
1:A:115:GLU:HG3	1:A:116:PRO:HD2	1.36	1.03
1:C:312:LEU:HD12	1:C:317:VAL:HG21	1.36	1.02
2:F:541:LYS:CB	2:F:587:GLN:OE1	2.06	1.02
2:H:440:ILE:CB	2:H:462:GLY:HA3	1.90	1.02
1:A:118:LYS:HE3	1:A:119:PRO:CG	1.88	1.02
1:C:391:ILE:HD12	1:C:391:ILE:H	1.24	1.01
2:E:541:LYS:CG	2:E:587:GLN:CD	2.31	1.01
1:A:115:GLU:CG	1:A:116:PRO:CD	2.39	1.01
1:B:118:LYS:HE3	1:B:119:PRO:CG	1.89	1.01
2:F:541:LYS:CG	2:F:587:GLN:CD	2.33	1.01
2:G:440:ILE:CB	2:G:462:GLY:HA3	1.90	1.01
2:F:541:LYS:HE2	2:F:587:GLN:HE22	1.26	1.01
2:G:456:LEU:HD21	2:G:501:LYS:HE2	1.43	1.01
1:C:252:LYS:HE2	1:C:274:VAL:HG23	1.38	1.00
2:H:456:LEU:HD21	2:H:501:LYS:HE2	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:541:LYS:HE2	2:E:587:GLN:HE22	1.26	0.98
2:F:479:VAL:HG21	2:F:504:LEU:HD23	1.44	0.98
1:A:91:ASN:O	1:A:120:ILE:CG2	2.12	0.97
1:D:252:LYS:CE	1:D:274:VAL:CG2	2.43	0.96
2:E:473:MET:HE1	2:E:525:CYS:O	1.64	0.96
2:E:479:VAL:HG21	2:E:504:LEU:HD23	1.47	0.96
1:B:115:GLU:CG	1:B:116:PRO:CD	2.39	0.96
1:D:291:PHE:HE1	1:D:401:GLN:NE2	1.63	0.96
1:B:91:ASN:O	1:B:120:ILE:CG2	2.13	0.96
2:G:530:THR:O	2:G:633:VAL:HG23	1.66	0.95
1:C:252:LYS:CE	1:C:274:VAL:CG2	2.44	0.95
1:C:291:PHE:HE1	1:C:401:GLN:NE2	1.62	0.95
2:G:541:LYS:CG	2:G:587:GLN:CD	2.36	0.95
2:H:633:VAL:CG1	2:H:634:PRO:CD	2.37	0.95
1:C:252:LYS:CE	1:C:274:VAL:HG23	1.96	0.95
2:E:489:VAL:HG12	2:E:490:GLU:N	1.81	0.95
1:B:118:LYS:CE	1:B:119:PRO:CD	2.37	0.95
1:D:252:LYS:CE	1:D:274:VAL:HG23	1.96	0.95
1:B:118:LYS:CD	1:B:119:PRO:CD	2.45	0.94
1:B:118:LYS:HD2	1:B:119:PRO:HD3	1.47	0.94
2:E:541:LYS:CG	2:E:587:GLN:HE22	1.72	0.94
2:F:489:VAL:HG12	2:F:490:GLU:N	1.83	0.94
2:G:633:VAL:CG1	2:G:634:PRO:CD	2.37	0.94
2:H:541:LYS:CG	2:H:587:GLN:CD	2.38	0.93
1:A:347:THR:CB	1:A:348:PRO:HD2	1.97	0.93
1:A:118:LYS:HE3	1:A:119:PRO:HD3	1.28	0.93
2:H:530:THR:O	2:H:633:VAL:HG23	1.67	0.93
1:B:347:THR:CB	1:B:348:PRO:HD2	1.99	0.93
2:F:545:CYS:CB	2:F:546:PRO:HD2	1.97	0.93
1:A:118:LYS:CD	1:A:119:PRO:CD	2.46	0.92
2:H:440:ILE:HB	2:H:462:GLY:CA	1.99	0.92
1:A:118:LYS:HD2	1:A:119:PRO:HD3	1.51	0.91
1:B:347:THR:HB	1:B:348:PRO:CD	2.00	0.91
2:G:440:ILE:HB	2:G:462:GLY:CA	1.99	0.91
1:A:114:PHE:CD1	1:A:115:GLU:O	2.24	0.91
1:A:41:PRO:O	1:A:42:LYS:HG2	1.71	0.91
1:B:114:PHE:CD1	1:B:115:GLU:O	2.24	0.91
1:B:115:GLU:HG2	1:B:116:PRO:HD2	1.53	0.90
2:H:489:VAL:HG12	2:H:490:GLU:N	1.85	0.90
1:A:347:THR:HB	1:A:348:PRO:CD	1.98	0.90
1:A:115:GLU:HG2	1:A:116:PRO:HD2	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:541:LYS:HG2	2:G:587:GLN:HE22	1.10	0.90
1:B:223:GLY:O	1:B:249:LYS:O	1.90	0.90
2:E:489:VAL:HG12	2:E:490:GLU:H	1.36	0.90
2:G:489:VAL:HG12	2:G:490:GLU:H	1.35	0.90
1:B:118:LYS:CG	1:B:119:PRO:CD	2.50	0.90
1:A:118:LYS:CG	1:A:119:PRO:CD	2.50	0.89
2:H:489:VAL:HG12	2:H:490:GLU:H	1.34	0.89
2:G:489:VAL:HG12	2:G:490:GLU:N	1.85	0.89
2:F:541:LYS:CG	2:F:587:GLN:HE22	1.75	0.88
2:H:541:LYS:HG2	2:H:587:GLN:HE22	1.08	0.88
2:E:541:LYS:HE2	2:E:587:GLN:NE2	1.89	0.88
2:H:541:LYS:CD	2:H:587:GLN:HE22	1.86	0.88
2:E:473:MET:CE	2:E:525:CYS:O	2.22	0.88
2:F:489:VAL:HG12	2:F:490:GLU:H	1.38	0.88
1:A:223:GLY:O	1:A:249:LYS:O	1.91	0.87
2:G:521:PRO:HB2	2:G:522:ASN:HB2	1.56	0.87
2:F:521:PRO:HB2	2:F:522:ASN:HB2	1.56	0.86
2:G:541:LYS:CD	2:G:587:GLN:HE22	1.87	0.86
1:C:317:VAL:HG12	1:C:413:LEU:HD23	1.57	0.86
1:B:231:ASP:O	1:B:235:GLU:HB2	1.76	0.86
1:B:41:PRO:O	1:B:42:LYS:HG2	1.76	0.86
1:C:245:ARG:H	1:C:245:ARG:HD2	1.40	0.86
2:E:521:PRO:HB2	2:E:522:ASN:HB2	1.56	0.86
1:A:231:ASP:O	1:A:235:GLU:HB2	1.76	0.85
2:G:541:LYS:CG	2:G:587:GLN:OE1	2.22	0.85
2:H:521:PRO:HB2	2:H:522:ASN:HB2	1.56	0.85
1:A:107:GLU:O	1:A:108:LYS:HB2	1.77	0.85
1:D:315:GLY:HA3	1:D:415:TYR:OH	1.75	0.85
2:E:529:ARG:HA	2:E:597:THR:CG2	2.07	0.85
2:F:541:LYS:HE2	2:F:587:GLN:NE2	1.91	0.85
2:F:447:LYS:HG3	2:F:512:ILE:HG23	1.56	0.85
1:D:245:ARG:H	1:D:245:ARG:HD2	1.40	0.85
1:B:245:ARG:H	1:B:245:ARG:HD2	1.42	0.84
1:C:347:THR:HB	1:C:348:PRO:CD	2.08	0.84
1:B:107:GLU:O	1:B:108:LYS:HB2	1.77	0.84
2:H:603:LEU:O	2:H:604:GLU:HG2	1.78	0.84
2:G:633:VAL:CB	2:G:634:PRO:CD	2.56	0.84
2:E:447:LYS:HG3	2:E:512:ILE:HG23	1.57	0.84
1:D:347:THR:HB	1:D:348:PRO:CD	2.08	0.84
2:G:558:ILE:O	2:G:559:GLU:HB2	1.78	0.84
1:B:300:LYS:O	1:B:413:LEU:N	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:603:LEU:O	2:G:604:GLU:HG2	1.78	0.83
1:B:118:LYS:CG	1:B:119:PRO:HD2	2.08	0.83
1:B:316:ALA:HB1	1:B:386:GLY:HA3	1.61	0.83
1:C:291:PHE:HE1	1:C:401:GLN:HE21	1.21	0.83
2:E:473:MET:HB3	2:E:474:PRO:HD3	1.58	0.83
2:G:495:ALA:HB1	2:G:496:PRO:HD2	1.61	0.83
1:A:118:LYS:HG3	1:A:119:PRO:HD2	1.61	0.82
2:H:633:VAL:CB	2:H:634:PRO:CD	2.56	0.82
2:G:633:VAL:HB	2:G:634:PRO:HD2	1.61	0.82
2:H:444:ILE:CG2	2:H:455:VAL:HG13	2.09	0.82
2:H:633:VAL:HB	2:H:634:PRO:HD2	1.62	0.82
1:B:118:LYS:HG3	1:B:119:PRO:HD2	1.60	0.82
2:H:558:ILE:O	2:H:559:GLU:HB2	1.78	0.82
1:D:291:PHE:HE1	1:D:401:GLN:HE21	1.22	0.82
2:H:541:LYS:CG	2:H:587:GLN:OE1	2.27	0.82
2:H:545:CYS:CB	2:H:546:PRO:HD2	1.99	0.82
1:B:92:GLY:HA3	1:B:120:ILE:CG2	2.10	0.82
1:A:316:ALA:HB1	1:A:386:GLY:HA3	1.62	0.81
1:C:223:GLY:O	1:C:249:LYS:O	1.99	0.81
2:G:444:ILE:CG2	2:G:455:VAL:HG13	2.08	0.81
1:A:118:LYS:CE	1:A:119:PRO:CD	2.35	0.81
1:A:118:LYS:CG	1:A:119:PRO:HD2	2.11	0.81
2:F:473:MET:HB3	2:F:474:PRO:HD3	1.63	0.81
1:A:92:GLY:HA3	1:A:120:ILE:CG2	2.11	0.81
2:F:447:LYS:O	2:F:448:TYR:HB3	1.81	0.81
2:H:495:ALA:HB1	2:H:496:PRO:HD2	1.61	0.81
1:A:118:LYS:CG	1:A:119:PRO:HD3	2.10	0.81
1:D:223:GLY:O	1:D:249:LYS:O	1.99	0.81
2:F:545:CYS:HB2	2:F:546:PRO:CD	2.06	0.80
1:B:291:PHE:HE2	1:B:406:PHE:HE1	1.28	0.80
2:E:540:HIS:NE2	2:E:543:ILE:O	2.14	0.80
1:A:245:ARG:H	1:A:245:ARG:HD2	1.43	0.80
1:C:315:GLY:HA3	1:C:415:TYR:OH	1.80	0.80
2:H:441:ARG:CG	2:H:525:CYS:SG	2.70	0.80
2:E:541:LYS:CG	2:E:587:GLN:OE1	2.28	0.80
1:B:176:LEU:O	1:B:178:LYS:N	2.15	0.79
1:A:176:LEU:O	1:A:178:LYS:N	2.15	0.79
2:F:540:HIS:NE2	2:F:543:ILE:O	2.15	0.79
1:A:291:PHE:HE2	1:A:406:PHE:HE1	1.27	0.79
2:H:441:ARG:HD3	2:H:525:CYS:SG	2.23	0.79
1:A:118:LYS:HE3	1:A:119:PRO:HG3	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:545:CYS:HB2	2:E:546:PRO:CD	2.05	0.79
1:C:195:MET:HA	1:C:198:ARG:HB3	1.65	0.78
2:E:545:CYS:CB	2:E:546:PRO:HD2	1.96	0.78
2:G:441:ARG:HD3	2:G:525:CYS:SG	2.24	0.78
2:H:530:THR:C	2:H:633:VAL:HG23	2.09	0.78
1:B:118:LYS:HE3	1:B:119:PRO:HG3	1.63	0.78
1:C:317:VAL:HG12	1:C:413:LEU:CD2	2.14	0.78
2:F:524:LEU:HD12	2:F:525:CYS:H	1.46	0.78
2:G:441:ARG:CG	2:G:525:CYS:SG	2.72	0.78
2:H:555:HIS:C	2:H:557:CYS:H	1.90	0.78
1:A:300:LYS:O	1:A:413:LEU:N	2.16	0.78
2:G:530:THR:C	2:G:633:VAL:HG23	2.08	0.78
2:E:447:LYS:O	2:E:448:TYR:HB3	1.83	0.77
1:B:118:LYS:CG	1:B:119:PRO:HD3	2.12	0.77
2:E:453:THR:OG1	2:E:509:GLU:HB3	1.84	0.77
2:H:540:HIS:NE2	2:H:543:ILE:O	2.17	0.77
2:E:473:MET:HG2	2:E:602:CYS:CB	2.12	0.77
2:F:606:PHE:H	2:F:629:VAL:HG13	1.50	0.77
2:G:489:VAL:CG1	2:G:490:GLU:H	1.97	0.77
2:G:545:CYS:CB	2:G:546:PRO:HD2	1.98	0.77
1:D:195:MET:HA	1:D:198:ARG:HB3	1.65	0.77
2:E:473:MET:HG2	2:E:602:CYS:HB3	1.64	0.77
2:G:456:LEU:CD2	2:G:501:LYS:HG2	2.15	0.77
2:G:546:PRO:HD2	2:G:583:ARG:O	1.84	0.77
1:A:81:ARG:HD2	1:A:111:ASN:HB3	1.65	0.77
1:A:275:LEU:C	1:A:277:ASN:H	1.90	0.77
2:G:555:HIS:C	2:G:557:CYS:H	1.91	0.77
1:B:81:ARG:HD2	1:B:111:ASN:HB3	1.66	0.77
1:B:120:ILE:HD12	1:B:121:ASN:H	1.50	0.77
2:H:489:VAL:CG1	2:H:490:GLU:H	1.96	0.77
2:F:541:LYS:CG	2:F:587:GLN:OE1	2.30	0.77
2:H:546:PRO:HD2	2:H:583:ARG:O	1.84	0.77
1:A:279:LYS:H	1:A:279:LYS:HD3	1.49	0.77
1:B:275:LEU:C	1:B:277:ASN:H	1.92	0.77
2:F:453:THR:OG1	2:F:509:GLU:HB3	1.84	0.76
2:G:540:HIS:NE2	2:G:543:ILE:O	2.18	0.76
2:H:530:THR:HG22	2:H:633:VAL:HG21	1.67	0.76
2:H:633:VAL:HG12	2:H:634:PRO:HD3	0.81	0.76
2:E:541:LYS:CD	2:E:587:GLN:NE2	2.40	0.76
2:E:606:PHE:H	2:E:629:VAL:HG13	1.50	0.76
2:H:510:GLU:HG3	2:H:511:GLU:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:456:LEU:CD2	2:H:501:LYS:HG2	2.16	0.76
1:A:120:ILE:HD12	1:A:121:ASN:H	1.51	0.76
2:G:473:MET:HE2	2:G:525:CYS:O	1.86	0.76
1:A:114:PHE:HD1	1:A:115:GLU:O	1.69	0.75
1:B:279:LYS:HD3	1:B:279:LYS:H	1.49	0.75
2:F:494:VAL:HG21	2:F:500:LEU:HD11	1.68	0.75
2:H:441:ARG:HG2	2:H:525:CYS:SG	2.25	0.75
1:A:118:LYS:CB	1:A:119:PRO:CD	2.64	0.75
1:B:118:LYS:CB	1:B:119:PRO:CD	2.64	0.75
2:G:541:LYS:CE	2:G:587:GLN:HE22	2.00	0.75
2:G:456:LEU:HD21	2:G:501:LYS:CE	2.17	0.75
2:F:473:MET:HG2	2:F:602:CYS:HB3	1.67	0.75
2:G:530:THR:HG22	2:G:633:VAL:HG21	1.69	0.75
2:H:473:MET:HE2	2:H:525:CYS:O	1.87	0.75
1:A:275:LEU:O	1:A:277:ASN:N	2.18	0.74
2:G:510:GLU:HG3	2:G:511:GLU:H	1.52	0.74
1:B:316:ALA:CB	1:B:386:GLY:HA3	2.17	0.74
2:F:473:MET:HG2	2:F:602:CYS:CB	2.17	0.74
2:F:543:ILE:HG22	2:F:544:ILE:N	2.02	0.74
2:G:441:ARG:HG2	2:G:525:CYS:SG	2.28	0.74
2:F:469:GLN:OE1	2:F:480:GLU:HB2	1.88	0.74
1:D:75:ILE:O	1:D:78:VAL:HG12	1.87	0.74
1:B:115:GLU:HG3	1:B:116:PRO:HD3	1.69	0.73
2:H:541:LYS:CE	2:H:587:GLN:HE22	2.01	0.73
1:C:252:LYS:CE	1:C:274:VAL:HG21	2.12	0.73
1:A:316:ALA:CB	1:A:386:GLY:HA3	2.18	0.73
1:B:114:PHE:HD1	1:B:115:GLU:O	1.70	0.73
2:F:553:HIS:HB2	2:F:616:THR:HG23	1.69	0.73
2:E:494:VAL:HG21	2:E:500:LEU:HD11	1.71	0.73
1:D:195:MET:HG2	1:D:198:ARG:HH11	1.52	0.73
2:H:456:LEU:HD21	2:H:501:LYS:CE	2.18	0.73
2:E:469:GLN:OE1	2:E:480:GLU:HB2	1.88	0.73
2:E:543:ILE:HG22	2:E:544:ILE:N	2.03	0.73
1:C:195:MET:HG2	1:C:198:ARG:HH11	1.54	0.72
2:G:545:CYS:HB2	2:G:583:ARG:O	1.90	0.72
1:B:275:LEU:O	1:B:277:ASN:N	2.22	0.72
1:C:75:ILE:O	1:C:78:VAL:HG12	1.88	0.72
2:F:541:LYS:CD	2:F:587:GLN:NE2	2.44	0.72
2:G:573:LYS:O	2:G:573:LYS:HG3	1.90	0.72
2:H:537:ILE:HG21	2:H:587:GLN:HA	1.71	0.72
2:G:456:LEU:CD2	2:G:501:LYS:HE2	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:HG3	1:A:116:PRO:HD3	1.70	0.71
2:H:633:VAL:CB	2:H:634:PRO:HD2	2.19	0.71
2:H:489:VAL:CG1	2:H:490:GLU:N	2.53	0.71
2:E:553:HIS:HB2	2:E:616:THR:HG23	1.71	0.71
2:F:530:THR:HB	2:F:633:VAL:O	1.91	0.71
1:C:291:PHE:CE1	1:C:401:GLN:NE2	2.54	0.71
2:H:456:LEU:CD2	2:H:501:LYS:HE2	2.20	0.71
2:H:444:ILE:HG23	2:H:455:VAL:CG1	2.19	0.71
2:H:545:CYS:HB2	2:H:583:ARG:O	1.89	0.71
1:D:252:LYS:CE	1:D:274:VAL:HG21	2.11	0.71
2:E:489:VAL:CG1	2:E:490:GLU:N	2.54	0.71
2:F:473:MET:HE2	2:F:525:CYS:O	1.90	0.71
1:A:38:ILE:HD12	1:A:124:LEU:HD13	1.73	0.71
1:A:276:SER:HA	1:A:279:LYS:HE3	1.72	0.70
2:G:633:VAL:CB	2:G:634:PRO:HD2	2.20	0.70
2:G:545:CYS:HB2	2:G:546:PRO:CD	2.12	0.70
1:C:152:ASP:OD1	1:C:258:TYR:O	2.10	0.70
2:E:489:VAL:CG1	2:E:490:GLU:H	2.04	0.70
2:F:489:VAL:CG1	2:F:490:GLU:N	2.55	0.70
1:D:291:PHE:CE1	1:D:401:GLN:NE2	2.55	0.70
2:G:633:VAL:HG12	2:G:634:PRO:HD3	0.81	0.70
2:G:444:ILE:HG23	2:G:455:VAL:CG1	2.17	0.70
1:B:276:SER:HA	1:B:279:LYS:HE3	1.71	0.70
2:H:573:LYS:HG3	2:H:573:LYS:O	1.92	0.70
2:G:447:LYS:HG3	2:G:512:ILE:HG23	1.74	0.70
2:G:543:ILE:HG22	2:G:544:ILE:N	2.07	0.70
1:A:118:LYS:HE2	3:A:1526:ATP:PG	2.31	0.69
2:E:444:ILE:HG23	2:E:455:VAL:HG13	1.74	0.69
2:F:444:ILE:HG23	2:F:455:VAL:HG13	1.74	0.69
2:G:447:LYS:O	2:G:448:TYR:HB3	1.92	0.69
2:H:486:SER:HA	2:H:500:LEU:HD12	1.73	0.69
2:G:554:ILE:HD12	2:G:601:ILE:HG21	1.74	0.69
2:H:537:ILE:CG2	2:H:587:GLN:HA	2.23	0.69
2:G:533:ALA:O	2:G:592:ILE:HA	1.92	0.69
1:D:283:GLU:HG3	1:D:392:VAL:HG12	1.75	0.69
2:G:486:SER:HA	2:G:500:LEU:HD12	1.74	0.69
2:H:533:ALA:O	2:H:592:ILE:HA	1.93	0.69
2:H:447:LYS:O	2:H:448:TYR:HB3	1.92	0.69
2:H:554:ILE:HD12	2:H:601:ILE:HG21	1.75	0.69
1:D:152:ASP:OD1	1:D:258:TYR:O	2.11	0.69
2:G:537:ILE:HG21	2:G:587:GLN:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:GLN:C	1:D:399:GLY:H	2.00	0.68
2:H:543:ILE:HG22	2:H:544:ILE:N	2.09	0.68
2:F:529:ARG:H	2:F:529:ARG:HD3	1.56	0.68
1:B:13:GLU:OE1	1:B:13:GLU:HA	1.91	0.68
2:E:530:THR:HB	2:E:633:VAL:O	1.93	0.68
2:E:540:HIS:CG	2:E:542:SER:H	2.12	0.68
2:G:489:VAL:CG1	2:G:490:GLU:N	2.53	0.68
1:A:277:ASN:O	1:A:280:PHE:HB2	1.94	0.68
1:B:38:ILE:HD12	1:B:124:LEU:HD13	1.75	0.68
1:B:305:VAL:HG23	1:B:306:GLU:N	2.09	0.68
2:G:536:VAL:HG22	2:G:536:VAL:O	1.92	0.68
1:B:91:ASN:HB2	1:B:116:PRO:HD2	1.76	0.68
1:D:156:ALA:HB2	1:D:201:TYR:OH	1.94	0.68
1:B:91:ASN:HB3	1:B:119:PRO:HA	1.75	0.68
1:A:91:ASN:HB3	1:A:119:PRO:HA	1.75	0.68
1:B:327:ASP:HB3	1:B:347:THR:CG2	2.23	0.68
2:E:529:ARG:HA	2:E:597:THR:HG22	1.76	0.68
1:C:233:LYS:O	1:C:237:SER:HB2	1.93	0.67
2:E:554:ILE:HG23	2:E:615:PHE:HB3	1.77	0.67
2:E:464:ILE:HG23	2:E:494:VAL:CG1	2.25	0.67
2:F:568:CYS:HB2	2:F:592:ILE:HD11	1.75	0.67
1:A:92:GLY:HA3	1:A:120:ILE:HG21	1.77	0.67
1:A:13:GLU:HA	1:A:13:GLU:OE1	1.94	0.67
2:F:489:VAL:CG1	2:F:490:GLU:H	2.05	0.67
2:G:537:ILE:CG2	2:G:587:GLN:HA	2.25	0.67
1:A:305:VAL:HG23	1:A:306:GLU:N	2.09	0.67
1:B:277:ASN:O	1:B:280:PHE:HB2	1.94	0.67
1:D:118:LYS:HE2	1:D:120:ILE:HG12	1.77	0.67
2:F:464:ILE:HG23	2:F:494:VAL:CG1	2.24	0.67
1:C:397:GLN:C	1:C:399:GLY:H	2.00	0.67
1:D:233:LYS:O	1:D:237:SER:HB2	1.94	0.67
2:F:540:HIS:CG	2:F:542:SER:H	2.12	0.67
2:F:573:LYS:HG3	2:F:573:LYS:O	1.95	0.67
2:G:553:HIS:HB2	2:G:616:THR:HG23	1.77	0.67
2:H:447:LYS:HG3	2:H:512:ILE:HG23	1.76	0.67
2:E:473:MET:CB	2:E:474:PRO:HD3	2.24	0.67
1:C:378:PHE:O	1:C:382:TYR:HB3	1.95	0.66
1:B:92:GLY:HA3	1:B:120:ILE:HG21	1.75	0.66
1:C:312:LEU:HD12	1:C:317:VAL:CG2	2.21	0.66
2:G:467:GLY:HA2	2:G:481:VAL:O	1.96	0.66
2:G:540:HIS:CE1	2:G:542:SER:OG	2.48	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HD12	1:A:171:LYS:HD3	1.78	0.66
1:A:327:ASP:HB3	1:A:347:THR:CG2	2.24	0.66
2:F:554:ILE:HG23	2:F:615:PHE:HB3	1.78	0.66
1:C:283:GLU:HG3	1:C:392:VAL:HG12	1.76	0.66
2:H:467:GLY:HA2	2:H:481:VAL:O	1.96	0.66
2:H:536:VAL:HG22	2:H:536:VAL:O	1.95	0.66
1:D:378:PHE:O	1:D:382:TYR:HB3	1.95	0.66
2:F:546:PRO:HD2	2:F:583:ARG:O	1.96	0.66
2:G:440:ILE:O	2:G:440:ILE:HG13	1.95	0.66
1:A:91:ASN:HB2	1:A:116:PRO:HD2	1.76	0.66
1:C:156:ALA:HB2	1:C:201:TYR:OH	1.95	0.66
1:B:120:ILE:HD12	1:B:121:ASN:N	2.10	0.65
2:H:553:HIS:HB2	2:H:616:THR:HG23	1.79	0.65
1:A:146:PHE:CE2	1:A:275:LEU:HG	2.30	0.65
2:F:539:GLU:O	2:F:624:ILE:HA	1.96	0.65
2:H:540:HIS:CE1	2:H:542:SER:OG	2.49	0.65
2:E:573:LYS:O	2:E:573:LYS:HG3	1.95	0.65
2:H:633:VAL:CG1	2:H:634:PRO:HD2	2.26	0.65
1:A:120:ILE:HD12	1:A:121:ASN:N	2.11	0.65
1:B:146:PHE:CE2	1:B:275:LEU:HG	2.32	0.64
1:D:151:ILE:CG2	1:D:232:PHE:HB3	2.27	0.64
2:E:473:MET:CG	2:E:602:CYS:HB3	2.26	0.64
2:E:568:CYS:HB2	2:E:592:ILE:HD11	1.78	0.64
1:A:177:PRO:HG2	1:A:193:LEU:HD22	1.79	0.64
1:A:382:TYR:HE1	1:A:388:THR:HA	1.63	0.64
1:C:118:LYS:HE2	1:C:120:ILE:HG12	1.79	0.64
2:G:517:ILE:HG12	2:G:602:CYS:SG	2.36	0.64
2:E:521:PRO:HB2	2:E:522:ASN:CB	2.26	0.64
2:H:441:ARG:CD	2:H:525:CYS:SG	2.84	0.64
2:H:555:HIS:C	2:H:557:CYS:N	2.56	0.64
2:G:626:ILE:CG2	2:G:627:GLY:N	2.61	0.64
1:B:141:SER:O	1:B:143:ASP:N	2.30	0.64
2:F:551:VAL:HG12	2:F:558:ILE:HD11	1.80	0.64
1:C:76:THR:O	1:C:80:GLN:HG2	1.98	0.64
2:F:464:ILE:HG23	2:F:494:VAL:HG13	1.77	0.63
2:F:561:VAL:HG23	2:F:596:ARG:O	1.97	0.63
1:B:157:LEU:HD12	1:B:171:LYS:HD3	1.80	0.63
2:E:464:ILE:HG23	2:E:494:VAL:HG13	1.79	0.63
2:F:521:PRO:HB2	2:F:522:ASN:CB	2.26	0.63
2:H:440:ILE:O	2:H:440:ILE:HG13	1.97	0.63
2:H:510:GLU:HG3	2:H:511:GLU:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:545:CYS:HB2	2:H:546:PRO:CD	2.12	0.63
1:B:10:ARG:O	1:B:13:GLU:HB2	1.98	0.63
2:G:555:HIS:C	2:G:557:CYS:N	2.57	0.63
2:H:517:ILE:HG12	2:H:602:CYS:SG	2.38	0.63
2:E:546:PRO:HD2	2:E:583:ARG:O	1.98	0.63
2:F:473:MET:CB	2:F:474:PRO:HD3	2.28	0.63
2:G:633:VAL:CG1	2:G:634:PRO:HD2	2.28	0.63
1:A:10:ARG:O	1:A:13:GLU:HB2	1.98	0.63
1:A:121:ASN:C	1:A:122:THR:HG22	2.24	0.63
1:D:317:VAL:HG12	1:D:413:LEU:HD23	1.80	0.63
1:B:95:VAL:HG13	1:B:113:ASP:HB3	1.80	0.63
1:B:177:PRO:HG2	1:B:193:LEU:HD22	1.81	0.63
1:B:382:TYR:HE1	1:B:388:THR:HA	1.63	0.63
1:C:151:ILE:CG2	1:C:232:PHE:HB3	2.29	0.62
1:D:76:THR:O	1:D:80:GLN:HG2	1.98	0.62
2:G:456:LEU:HG	2:G:501:LYS:HG2	1.80	0.62
2:F:473:MET:CG	2:F:602:CYS:HB3	2.29	0.62
2:F:554:ILE:HB	2:F:557:CYS:SG	2.40	0.62
2:G:441:ARG:CD	2:G:525:CYS:SG	2.86	0.62
2:G:510:GLU:HG3	2:G:511:GLU:N	2.14	0.62
1:B:121:ASN:C	1:B:122:THR:HG22	2.24	0.62
2:F:559:GLU:HG3	2:F:560:GLU:N	2.13	0.62
2:H:464:ILE:HG23	2:H:494:VAL:HG13	1.81	0.62
1:B:326:LEU:HD21	1:B:328:ILE:HD12	1.80	0.62
1:C:166:ARG:H	1:C:166:ARG:HE	1.47	0.62
2:F:508:GLU:HB3	2:F:511:GLU:HB2	1.80	0.62
2:F:564:THR:OG1	2:F:594:ARG:HB3	2.00	0.62
2:H:456:LEU:HG	2:H:501:LYS:HG2	1.80	0.62
2:E:554:ILE:HB	2:E:557:CYS:SG	2.40	0.62
1:A:141:SER:O	1:A:143:ASP:N	2.32	0.62
1:A:214:ILE:HD12	1:A:245:ARG:HD3	1.82	0.62
1:D:391:ILE:H	1:D:391:ILE:CD1	1.92	0.62
2:E:540:HIS:CE1	2:E:542:SER:OG	2.53	0.62
2:G:540:HIS:CB	2:G:541:LYS:CA	2.37	0.62
1:A:291:PHE:CE2	1:A:406:PHE:HE1	2.14	0.62
2:E:508:GLU:HB3	2:E:511:GLU:HB2	1.81	0.62
2:F:473:MET:SD	2:F:525:CYS:HB2	2.39	0.62
2:G:533:ALA:CB	2:G:629:VAL:HA	2.30	0.62
1:A:190:PHE:O	1:A:194:ARG:HB2	2.00	0.61
1:B:190:PHE:O	1:B:194:ARG:HB2	2.00	0.61
1:B:233:LYS:HD2	1:B:253:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:O	1:A:25:GLU:HG2	2.01	0.61
1:A:233:LYS:HE3	1:A:254:VAL:O	2.00	0.61
1:D:166:ARG:H	1:D:166:ARG:HE	1.49	0.61
2:E:559:GLU:HG3	2:E:560:GLU:N	2.14	0.61
2:F:540:HIS:CB	2:F:541:LYS:CA	2.37	0.61
2:H:540:HIS:CG	2:H:542:SER:H	2.17	0.61
1:B:116:PRO:C	1:B:118:LYS:N	2.58	0.61
2:E:606:PHE:N	2:E:629:VAL:HG13	2.15	0.61
2:H:626:ILE:CG2	2:H:627:GLY:N	2.61	0.61
1:D:312:LEU:HD12	1:D:317:VAL:CG2	2.22	0.61
2:F:441:ARG:CZ	2:F:525:CYS:SG	2.88	0.61
2:G:521:PRO:HB2	2:G:522:ASN:CB	2.30	0.61
1:C:284:LYS:HG2	1:C:396:SER:HB2	1.83	0.61
2:G:464:ILE:HG23	2:G:494:VAL:HG13	1.81	0.61
2:H:521:PRO:HB2	2:H:522:ASN:CB	2.31	0.61
1:A:326:LEU:HD21	1:A:328:ILE:HD12	1.81	0.61
1:B:22:LYS:O	1:B:25:GLU:HG2	2.01	0.61
1:B:291:PHE:CE2	1:B:406:PHE:HE1	2.15	0.61
1:D:252:LYS:HE3	1:D:274:VAL:HG23	1.83	0.61
1:D:284:LYS:HG2	1:D:396:SER:HB2	1.83	0.61
2:G:540:HIS:CG	2:G:542:SER:H	2.18	0.61
2:H:594:ARG:C	2:H:595:LEU:HD12	2.26	0.61
2:E:543:ILE:HG22	2:E:544:ILE:C	2.26	0.61
2:F:540:HIS:HB3	2:F:541:LYS:C	2.25	0.61
2:F:543:ILE:HG22	2:F:544:ILE:C	2.26	0.61
1:A:95:VAL:HG13	1:A:113:ASP:HB3	1.82	0.60
2:E:540:HIS:HB3	2:E:541:LYS:HA	0.68	0.60
2:E:495:ALA:HB1	2:E:496:PRO:HD2	1.83	0.60
1:A:327:ASP:O	1:A:347:THR:HA	2.02	0.60
1:B:233:LYS:HE3	1:B:254:VAL:O	2.01	0.60
2:E:484:ILE:HG12	2:E:502:ILE:HG23	1.84	0.60
1:A:118:LYS:HE2	3:A:1526:ATP:O2G	2.02	0.60
1:A:323:TYR:HA	1:A:392:VAL:O	2.02	0.60
1:D:391:ILE:HD12	1:D:391:ILE:N	2.05	0.60
2:E:544:ILE:HG12	2:E:548:TYR:CD1	2.35	0.60
2:E:615:PHE:CE1	2:E:627:GLY:HA3	2.37	0.60
2:F:447:LYS:HZ3	2:F:510:GLU:HB2	1.64	0.60
2:F:528:GLY:O	2:F:600:THR:HG23	2.02	0.60
1:A:116:PRO:C	1:A:118:LYS:H	2.09	0.60
2:H:533:ALA:CB	2:H:629:VAL:HA	2.31	0.60
1:B:190:PHE:O	1:B:194:ARG:CB	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ARG:O	1:D:249:LYS:HG2	2.01	0.60
2:E:494:VAL:HG23	2:E:498:GLU:OE1	2.02	0.60
2:H:540:HIS:HB3	2:H:541:LYS:HA	0.69	0.60
1:B:196:GLU:O	1:B:200:ASN:HB2	2.02	0.60
1:B:214:ILE:HD12	1:B:245:ARG:HD3	1.83	0.60
1:C:252:LYS:HE3	1:C:274:VAL:HG23	1.82	0.60
2:E:564:THR:OG1	2:E:594:ARG:HB3	2.02	0.60
2:E:609:PHE:HB3	2:E:611:GLN:HE22	1.67	0.60
1:A:27:ALA:HB1	1:A:100:ILE:HG21	1.83	0.60
1:A:196:GLU:O	1:A:200:ASN:HB2	2.01	0.60
1:B:116:PRO:C	1:B:118:LYS:H	2.09	0.60
1:A:152:ASP:OD1	1:A:153:GLY:N	2.35	0.59
1:A:190:PHE:O	1:A:194:ARG:CB	2.49	0.59
2:F:475:ASN:O	2:F:476:LYS:C	2.45	0.59
2:F:540:HIS:CE1	2:F:542:SER:OG	2.55	0.59
2:G:594:ARG:C	2:G:595:LEU:HD12	2.27	0.59
1:A:91:ASN:HB3	1:A:118:LYS:O	2.01	0.59
1:B:152:ASP:OD1	1:B:153:GLY:N	2.35	0.59
2:F:615:PHE:CE1	2:F:627:GLY:HA3	2.37	0.59
1:B:191:ALA:O	1:B:192:ARG:C	2.46	0.59
2:E:473:MET:SD	2:E:525:CYS:HB2	2.42	0.59
1:A:245:ARG:O	1:A:249:LYS:HG2	2.03	0.59
2:E:442:LEU:O	2:E:517:ILE:HA	2.03	0.59
1:C:245:ARG:O	1:C:249:LYS:HG2	2.01	0.59
1:D:294:ILE:C	1:D:296:GLN:H	2.09	0.59
2:F:442:LEU:HB3	2:F:518:LEU:HB2	1.85	0.59
2:H:520:ASP:CG	2:H:521:PRO:HD2	2.27	0.59
1:B:91:ASN:HB3	1:B:118:LYS:O	2.02	0.59
1:C:294:ILE:C	1:C:296:GLN:H	2.10	0.59
2:H:555:HIS:O	2:H:557:CYS:N	2.36	0.59
2:F:495:ALA:HB1	2:F:496:PRO:HD2	1.84	0.59
1:A:233:LYS:HD2	1:A:253:LEU:HD22	1.84	0.59
1:B:133:THR:HG22	1:B:136:LEU:HD12	1.84	0.59
2:E:540:HIS:HB3	2:E:541:LYS:C	2.25	0.59
2:F:484:ILE:HG12	2:F:502:ILE:HG23	1.84	0.59
2:F:529:ARG:HA	2:F:597:THR:CG2	2.33	0.59
2:E:447:LYS:HZ3	2:E:510:GLU:HB2	1.67	0.58
1:B:118:LYS:CB	1:B:119:PRO:HD2	2.32	0.58
2:E:520:ASP:CG	2:E:521:PRO:HD2	2.28	0.58
2:E:563:ILE:HG22	2:E:595:LEU:HG	1.86	0.58
2:G:540:HIS:HB3	2:G:541:LYS:HA	0.70	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ALA:O	1:A:192:ARG:C	2.47	0.58
1:B:116:PRO:O	1:B:118:LYS:N	2.36	0.58
1:B:400:SER:O	1:B:404:LYS:HB2	2.03	0.58
1:A:118:LYS:CB	1:A:119:PRO:HD2	2.33	0.58
2:F:445:VAL:HG22	2:F:556:THR:CG2	2.34	0.58
2:F:477:HIS:CE1	2:F:507:ILE:HB	2.38	0.58
2:F:540:HIS:CE1	2:F:542:SER:HG	2.21	0.58
2:H:545:CYS:CB	2:H:546:PRO:CD	2.78	0.58
1:B:186:SER:HB3	1:B:189:ARG:H	1.68	0.58
2:E:445:VAL:HG22	2:E:556:THR:CG2	2.33	0.58
2:E:477:HIS:CE1	2:E:507:ILE:HB	2.38	0.58
2:G:555:HIS:O	2:G:557:CYS:N	2.37	0.58
1:A:252:LYS:HG2	1:A:253:LEU:O	2.03	0.58
1:A:286:LEU:HD13	1:A:390:GLU:HG3	1.84	0.58
2:E:442:LEU:HB3	2:E:518:LEU:HB2	1.86	0.58
2:F:442:LEU:O	2:F:517:ILE:HA	2.03	0.58
2:F:540:HIS:CE1	2:F:624:ILE:HD11	2.39	0.58
1:B:327:ASP:O	1:B:347:THR:HA	2.04	0.58
2:E:551:VAL:HG12	2:E:558:ILE:HD11	1.83	0.58
2:F:606:PHE:N	2:F:629:VAL:HG13	2.16	0.58
2:H:506:GLY:HA3	2:H:509:GLU:CD	2.29	0.58
2:H:540:HIS:CB	2:H:541:LYS:CA	2.37	0.58
1:D:233:LYS:HE3	1:D:254:VAL:O	2.03	0.58
2:E:541:LYS:CB	2:E:587:GLN:CD	2.72	0.58
2:F:520:ASP:CG	2:F:521:PRO:HD2	2.29	0.58
1:B:252:LYS:HG2	1:B:253:LEU:O	2.04	0.58
2:E:540:HIS:CE1	2:E:543:ILE:O	2.57	0.58
2:F:563:ILE:HG22	2:F:595:LEU:HG	1.86	0.58
2:G:520:ASP:CG	2:G:521:PRO:HD2	2.28	0.58
2:G:506:GLY:HA3	2:G:509:GLU:CD	2.29	0.57
2:G:543:ILE:CG2	2:G:544:ILE:N	2.67	0.57
1:A:116:PRO:O	1:A:118:LYS:N	2.37	0.57
1:A:400:SER:O	1:A:404:LYS:HB2	2.03	0.57
1:B:286:LEU:HD13	1:B:390:GLU:HG3	1.85	0.57
1:D:151:ILE:HG22	1:D:232:PHE:CG	2.39	0.57
2:E:459:LEU:HD11	2:E:464:ILE:HG22	1.85	0.57
2:E:543:ILE:CG2	2:E:544:ILE:N	2.67	0.57
1:A:116:PRO:C	1:A:118:LYS:N	2.58	0.57
2:E:489:VAL:HG11	2:H:575:GLY:HA2	1.87	0.57
1:A:118:LYS:HG3	1:A:119:PRO:CD	2.27	0.57
1:A:126:LEU:HD13	1:A:132:HIS:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LYS:O	1:A:20:LEU:C	2.48	0.57
1:A:382:TYR:CE1	1:A:388:THR:HA	2.39	0.57
1:C:271:SER:O	1:C:272:THR:C	2.48	0.57
2:E:559:GLU:HG2	2:E:597:THR:OG1	2.04	0.57
2:F:540:HIS:CE1	2:F:543:ILE:O	2.58	0.57
2:F:544:ILE:HG12	2:F:548:TYR:CD1	2.40	0.57
1:B:27:ALA:HB1	1:B:100:ILE:HG21	1.85	0.57
1:C:224:LEU:O	1:C:250:VAL:HA	2.05	0.57
1:C:233:LYS:HE3	1:C:254:VAL:O	2.04	0.57
1:C:391:ILE:HD12	1:C:391:ILE:N	2.06	0.57
2:E:464:ILE:CD1	2:E:470:LEU:HD11	2.35	0.57
2:F:494:VAL:HG23	2:F:498:GLU:OE1	2.04	0.57
2:F:538:ILE:HG12	2:F:625:ALA:HA	1.87	0.57
2:F:609:PHE:HB3	2:F:611:GLN:HE22	1.69	0.57
2:G:543:ILE:HG22	2:G:544:ILE:C	2.29	0.57
1:A:186:SER:HB3	1:A:189:ARG:H	1.69	0.57
1:B:382:TYR:CE1	1:B:388:THR:HA	2.39	0.57
1:C:151:ILE:HG22	1:C:232:PHE:CG	2.39	0.57
1:D:323:TYR:CE2	1:D:394:ASP:HB3	2.40	0.57
2:F:464:ILE:HD11	2:F:470:LEU:HD11	1.87	0.57
2:F:540:HIS:HB3	2:F:541:LYS:HA	0.67	0.57
2:F:464:ILE:CD1	2:F:470:LEU:HD11	2.35	0.56
2:E:441:ARG:CZ	2:E:525:CYS:SG	2.93	0.56
2:E:539:GLU:O	2:E:624:ILE:HA	2.05	0.56
2:E:540:HIS:CE1	2:E:542:SER:HG	2.23	0.56
2:F:543:ILE:CG2	2:F:544:ILE:N	2.67	0.56
1:A:347:THR:O	1:A:349:GLU:N	2.34	0.56
1:B:126:LEU:HD13	1:B:132:HIS:CD2	2.40	0.56
2:F:489:VAL:HG11	2:G:575:GLY:HA2	1.87	0.56
2:G:533:ALA:HB2	2:G:629:VAL:HA	1.87	0.56
2:H:543:ILE:HG22	2:H:544:ILE:C	2.30	0.56
1:C:326:LEU:C	1:C:328:ILE:H	2.14	0.56
1:D:271:SER:O	1:D:273:GLU:N	2.38	0.56
2:F:467:GLY:H	2:F:481:VAL:HB	1.69	0.56
2:G:456:LEU:CG	2:G:501:LYS:HG2	2.35	0.56
1:B:117:PHE:CE1	1:B:139:LEU:HD22	2.40	0.56
1:B:323:TYR:HA	1:B:392:VAL:O	2.06	0.56
1:D:224:LEU:O	1:D:250:VAL:HA	2.05	0.56
2:E:467:GLY:H	2:E:481:VAL:HB	1.70	0.56
2:H:533:ALA:HB2	2:H:629:VAL:HA	1.88	0.56
1:A:305:VAL:HG23	1:A:306:GLU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LYS:O	1:B:20:LEU:C	2.48	0.56
1:B:245:ARG:O	1:B:249:LYS:HG2	2.05	0.56
2:F:529:ARG:HB2	2:F:597:THR:HG23	1.86	0.56
2:H:543:ILE:CG2	2:H:544:ILE:N	2.69	0.56
1:B:58:THR:C	1:B:60:SER:H	2.14	0.56
1:B:327:ASP:HB3	1:B:347:THR:HG22	1.87	0.56
1:B:394:ASP:C	1:B:395:LYS:HG2	2.31	0.56
1:C:318:GLU:O	1:C:388:THR:HB	2.06	0.56
2:E:561:VAL:HG23	2:E:596:ARG:O	2.05	0.56
1:A:394:ASP:C	1:A:395:LYS:HG2	2.30	0.56
2:F:454:VAL:HG12	2:F:455:VAL:N	2.21	0.56
2:G:456:LEU:HD21	2:G:501:LYS:HG2	1.88	0.56
2:H:536:VAL:O	2:H:537:ILE:C	2.48	0.56
1:C:271:SER:O	1:C:273:GLU:N	2.39	0.56
1:D:271:SER:O	1:D:272:THR:C	2.47	0.56
2:E:464:ILE:HD11	2:E:470:LEU:HD11	1.88	0.56
2:H:633:VAL:HB	2:H:634:PRO:CD	2.26	0.56
2:F:538:ILE:O	2:F:540:HIS:N	2.39	0.55
2:H:500:LEU:HD23	2:H:502:ILE:HD11	1.87	0.55
1:B:10:ARG:HA	1:B:13:GLU:HG2	1.89	0.55
1:B:176:LEU:O	1:B:178:LYS:HG3	2.06	0.55
1:C:264:PHE:O	1:C:268:ILE:HG13	2.07	0.55
2:F:545:CYS:CB	2:F:546:PRO:CD	2.77	0.55
2:H:456:LEU:CG	2:H:501:LYS:HG2	2.35	0.55
2:H:531:PHE:HA	2:H:633:VAL:CG2	2.35	0.55
1:A:38:ILE:HG22	1:A:38:ILE:O	2.06	0.55
1:C:233:LYS:O	1:C:237:SER:CB	2.54	0.55
1:A:117:PHE:CE1	1:A:139:LEU:HD22	2.42	0.55
1:B:378:PHE:O	1:B:382:TYR:HB3	2.07	0.55
2:G:500:LEU:HD23	2:G:502:ILE:HD11	1.87	0.55
2:G:536:VAL:O	2:G:537:ILE:C	2.49	0.55
1:A:133:THR:HG22	1:A:136:LEU:HD12	1.88	0.55
1:A:378:PHE:O	1:A:382:TYR:HB3	2.07	0.55
1:D:326:LEU:HD13	1:D:328:ILE:HD12	1.87	0.55
2:G:531:PHE:HA	2:G:633:VAL:CG2	2.36	0.55
1:B:305:VAL:HG23	1:B:306:GLU:H	1.68	0.55
1:B:347:THR:O	1:B:349:GLU:N	2.31	0.55
1:D:318:GLU:O	1:D:388:THR:HB	2.06	0.55
2:F:604:GLU:HG2	2:F:612:MET:HE2	1.87	0.55
2:G:571:ASP:OD2	2:G:573:LYS:HG2	2.07	0.55
2:H:455:VAL:HG22	2:H:512:ILE:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:531:PHE:HA	2:H:633:VAL:HG23	1.89	0.55
1:A:327:ASP:HB3	1:A:347:THR:HG22	1.88	0.55
2:E:538:ILE:O	2:E:540:HIS:N	2.40	0.55
1:A:10:ARG:HA	1:A:13:GLU:HG2	1.89	0.55
1:D:264:PHE:O	1:D:268:ILE:HG13	2.06	0.55
2:F:459:LEU:HD11	2:F:464:ILE:HG22	1.88	0.55
1:B:91:ASN:HB3	1:B:116:PRO:HG2	1.89	0.55
1:D:326:LEU:C	1:D:328:ILE:H	2.14	0.55
2:F:571:ASP:OD2	2:F:573:LYS:HG2	2.07	0.55
2:G:531:PHE:HA	2:G:633:VAL:HG23	1.89	0.55
1:B:162:GLN:O	1:B:164:ASN:N	2.40	0.54
1:C:264:PHE:CE1	1:C:268:ILE:HD11	2.42	0.54
2:E:604:GLU:HG2	2:E:612:MET:HE2	1.89	0.54
2:H:548:TYR:HB3	2:H:563:ILE:HD11	1.89	0.54
1:A:58:THR:C	1:A:60:SER:H	2.14	0.54
1:B:394:ASP:HB3	1:B:403:VAL:HG21	1.88	0.54
1:D:320:LEU:HD21	1:D:378:PHE:CD2	2.42	0.54
2:E:571:ASP:OD2	2:E:573:LYS:HG2	2.07	0.54
2:G:544:ILE:HG12	2:G:548:TYR:CD1	2.42	0.54
2:G:615:PHE:HE1	2:G:617:LEU:HD22	1.72	0.54
1:A:245:ARG:H	1:A:245:ARG:CD	2.18	0.54
1:C:326:LEU:HD13	1:C:328:ILE:HD12	1.89	0.54
2:G:541:LYS:CB	2:G:587:GLN:CD	2.75	0.54
2:G:585:VAL:HG13	2:G:585:VAL:O	2.06	0.54
2:H:442:LEU:HB2	2:H:459:LEU:HD23	1.88	0.54
2:E:529:ARG:HA	2:E:597:THR:HG21	1.90	0.54
2:H:585:VAL:HG13	2:H:585:VAL:O	2.06	0.54
1:D:145:LYS:HE2	1:D:162:GLN:HE21	1.72	0.54
2:E:473:MET:HE2	2:E:525:CYS:O	2.06	0.54
1:A:394:ASP:HB3	1:A:403:VAL:HG21	1.89	0.54
1:C:391:ILE:H	1:C:391:ILE:CD1	1.94	0.54
1:D:233:LYS:O	1:D:237:SER:CB	2.55	0.54
2:E:571:ASP:OD1	2:E:572:LYS:N	2.41	0.54
2:G:443:PRO:HA	2:G:517:ILE:HA	1.89	0.54
2:G:548:TYR:HB3	2:G:563:ILE:HD11	1.89	0.54
2:H:486:SER:OG	2:H:498:GLU:HB3	2.08	0.54
2:F:545:CYS:HB2	2:F:583:ARG:O	2.08	0.53
2:G:486:SER:OG	2:G:498:GLU:HB3	2.08	0.53
2:H:486:SER:OG	2:H:498:GLU:OE1	2.26	0.53
1:A:176:LEU:O	1:A:178:LYS:HG3	2.08	0.53
1:A:274:VAL:O	1:A:277:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:VAL:O	1:B:277:ASN:HB2	2.09	0.53
2:F:541:LYS:CB	2:F:587:GLN:CD	2.74	0.53
2:F:559:GLU:HG2	2:F:597:THR:OG1	2.07	0.53
2:G:633:VAL:HB	2:G:634:PRO:CD	2.25	0.53
2:H:456:LEU:HD21	2:H:501:LYS:HG2	1.89	0.53
1:A:91:ASN:C	1:A:120:ILE:HG22	2.20	0.53
2:F:548:TYR:HB3	2:F:563:ILE:HD11	1.90	0.53
1:A:91:ASN:HB3	1:A:116:PRO:HG2	1.90	0.53
1:C:145:LYS:HE2	1:C:162:GLN:HE21	1.72	0.53
2:F:571:ASP:OD1	2:F:572:LYS:N	2.41	0.53
1:B:67:ASN:O	1:B:71:VAL:HG23	2.08	0.53
1:C:346:LEU:HD11	1:C:350:GLN:HB3	1.90	0.53
2:H:615:PHE:HE1	2:H:617:LEU:HD22	1.73	0.53
1:C:323:TYR:CE2	1:C:394:ASP:HB3	2.43	0.53
1:D:397:GLN:C	1:D:399:GLY:N	2.64	0.53
2:E:536:VAL:HG12	2:E:626:ILE:O	2.08	0.53
2:H:454:VAL:HG12	2:H:455:VAL:N	2.23	0.53
2:H:455:VAL:HG22	2:H:512:ILE:HD11	1.90	0.53
1:A:133:THR:C	1:A:135:ALA:N	2.64	0.53
1:B:151:ILE:HG21	1:B:232:PHE:HB3	1.91	0.53
2:E:548:TYR:HB3	2:E:563:ILE:HD11	1.90	0.53
2:F:447:LYS:O	2:F:448:TYR:CB	2.53	0.53
2:G:626:ILE:HG22	2:G:627:GLY:N	2.24	0.53
2:H:486:SER:CB	2:H:498:GLU:OE1	2.57	0.53
2:G:455:VAL:HG22	2:G:512:ILE:HD11	1.91	0.53
1:D:310:LYS:O	1:D:314:MET:HG2	2.09	0.53
2:H:440:ILE:CG2	2:H:462:GLY:HA3	2.38	0.53
1:D:264:PHE:CE1	1:D:268:ILE:HD11	2.44	0.53
2:G:440:ILE:CG2	2:G:462:GLY:HA3	2.38	0.53
2:G:454:VAL:HG12	2:G:455:VAL:N	2.23	0.53
2:H:538:ILE:O	2:H:540:HIS:N	2.42	0.53
1:A:119:PRO:O	1:A:120:ILE:C	2.52	0.52
1:B:393:THR:HB	1:B:395:LYS:HG3	1.90	0.52
2:H:571:ASP:OD2	2:H:573:LYS:HG2	2.09	0.52
1:C:320:LEU:HD21	1:C:378:PHE:CD2	2.43	0.52
2:F:441:ARG:NH2	2:F:525:CYS:SG	2.82	0.52
2:E:454:VAL:HG12	2:E:455:VAL:N	2.24	0.52
2:E:520:ASP:OD1	2:E:522:ASN:ND2	2.39	0.52
2:G:538:ILE:O	2:G:540:HIS:N	2.42	0.52
2:H:484:ILE:CG2	2:H:500:LEU:HG	2.40	0.52
2:H:544:ILE:HG12	2:H:548:TYR:CD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PRO:O	1:B:120:ILE:C	2.53	0.52
2:E:540:HIS:CE1	2:E:624:ILE:HD11	2.45	0.52
2:G:459:LEU:HD11	2:G:464:ILE:HG22	1.90	0.52
2:G:484:ILE:CG2	2:G:500:LEU:HG	2.39	0.52
1:A:239:SER:C	1:A:241:MET:H	2.18	0.52
1:D:416:ARG:HH11	1:D:418:ASP:HA	1.75	0.52
2:E:472:MET:HG2	2:E:473:MET:H	1.73	0.52
2:E:545:CYS:HB2	2:E:583:ARG:O	2.09	0.52
2:G:486:SER:OG	2:G:498:GLU:OE1	2.28	0.52
2:G:578:SER:OG	2:G:579:LYS:N	2.41	0.52
2:G:611:GLN:H	2:G:611:GLN:CD	2.18	0.52
2:H:459:LEU:HD11	2:H:464:ILE:HG22	1.90	0.52
2:H:484:ILE:HG12	2:H:502:ILE:HD13	1.92	0.52
2:H:563:ILE:HG22	2:H:595:LEU:HG	1.91	0.52
1:A:151:ILE:HG21	1:A:232:PHE:HB3	1.92	0.52
1:C:79:GLN:HA	1:C:82:LEU:HB3	1.92	0.52
1:D:208:THR:HG22	1:D:212:LEU:HD23	1.91	0.52
1:D:346:LEU:HD11	1:D:350:GLN:HB3	1.90	0.52
2:F:558:ILE:O	2:F:558:ILE:HG13	2.10	0.52
2:G:442:LEU:HB2	2:G:459:LEU:HD23	1.90	0.52
1:A:275:LEU:C	1:A:277:ASN:N	2.57	0.52
2:F:540:HIS:ND1	2:F:624:ILE:HD11	2.25	0.52
2:H:443:PRO:HA	2:H:517:ILE:HA	1.91	0.52
1:A:67:ASN:O	1:A:71:VAL:HG23	2.10	0.52
1:A:110:VAL:CG2	1:A:112:ILE:HD11	2.40	0.52
1:B:118:LYS:CE	1:B:119:PRO:HG3	2.39	0.52
1:C:264:PHE:CZ	1:C:268:ILE:HD11	2.45	0.52
2:F:450:ASP:CG	2:F:451:MET:N	2.68	0.52
1:B:176:LEU:O	1:B:178:LYS:CG	2.58	0.52
1:B:239:SER:C	1:B:241:MET:H	2.18	0.52
1:A:14:ILE:HG23	1:A:140:LEU:HD22	1.91	0.52
1:B:117:PHE:CE1	1:B:139:LEU:O	2.63	0.52
1:B:244:GLN:HB3	1:B:245:ARG:HD2	1.92	0.52
2:F:472:MET:HG2	2:F:473:MET:H	1.75	0.52
2:F:540:HIS:HE2	2:F:544:ILE:HG13	1.74	0.52
1:C:252:LYS:HG2	1:C:253:LEU:O	2.10	0.51
2:E:477:HIS:HE1	2:E:508:GLU:H	1.57	0.51
2:E:529:ARG:CA	2:E:597:THR:HG22	2.38	0.51
2:G:530:THR:C	2:G:633:VAL:CG2	2.82	0.51
2:G:558:ILE:O	2:G:559:GLU:CB	2.54	0.51
1:A:170:HIS:CD2	1:A:208:THR:HG21	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:459:LEU:O	2:E:496:PRO:HA	2.10	0.51
2:E:540:HIS:HE2	2:E:544:ILE:HG13	1.76	0.51
2:G:455:VAL:HG22	2:G:512:ILE:CD1	2.39	0.51
2:G:486:SER:CB	2:G:498:GLU:OE1	2.58	0.51
2:H:611:GLN:CD	2:H:611:GLN:H	2.18	0.51
1:A:117:PHE:CE1	1:A:139:LEU:O	2.63	0.51
1:A:302:CYS:HB3	1:A:413:LEU:HD11	1.93	0.51
1:C:208:THR:HG22	1:C:212:LEU:HD23	1.92	0.51
2:F:477:HIS:HE1	2:F:508:GLU:H	1.58	0.51
2:G:605:THR:O	2:G:606:PHE:C	2.53	0.51
1:A:94:VAL:O	1:A:113:ASP:HA	2.10	0.51
1:A:176:LEU:O	1:A:178:LYS:CG	2.59	0.51
1:B:115:GLU:HG2	1:B:116:PRO:CD	2.27	0.51
2:G:495:ALA:HB1	2:G:496:PRO:CD	2.39	0.51
2:G:554:ILE:CD1	2:G:601:ILE:HG21	2.40	0.51
1:B:170:HIS:CD2	1:B:208:THR:HG21	2.46	0.51
2:H:484:ILE:HG23	2:H:500:LEU:HG	1.92	0.51
2:H:546:PRO:CD	2:H:583:ARG:O	2.57	0.51
1:D:81:ARG:HH21	1:D:84:LEU:HD11	1.76	0.51
2:F:441:ARG:NE	2:F:525:CYS:SG	2.83	0.51
2:F:460:GLU:HB3	2:F:611:GLN:HG3	1.93	0.51
2:G:484:ILE:HG12	2:G:502:ILE:HD13	1.92	0.51
2:G:538:ILE:O	2:G:539:GLU:C	2.52	0.51
2:H:538:ILE:O	2:H:539:GLU:C	2.54	0.51
1:A:322:VAL:O	1:A:391:ILE:HA	2.11	0.51
1:A:393:THR:HB	1:A:395:LYS:HG3	1.91	0.51
2:E:473:MET:HB3	2:E:474:PRO:CD	2.36	0.51
2:F:536:VAL:HG12	2:F:626:ILE:O	2.10	0.51
1:A:303:PHE:HD2	1:A:303:PHE:N	2.08	0.51
1:B:110:VAL:CG2	1:B:112:ILE:HD11	2.41	0.51
1:B:322:VAL:HG12	1:B:323:TYR:N	2.25	0.51
1:D:252:LYS:HG2	1:D:253:LEU:O	2.09	0.51
2:E:474:PRO:HG3	2:E:602:CYS:HB3	1.92	0.51
1:A:117:PHE:CZ	1:A:139:LEU:O	2.64	0.51
1:B:118:LYS:HB3	1:B:119:PRO:HD2	1.93	0.51
1:B:303:PHE:N	1:B:303:PHE:HD2	2.09	0.51
2:H:468:GLN:HB3	2:H:470:LEU:HD13	1.93	0.51
2:G:571:ASP:OD1	2:G:572:LYS:N	2.43	0.50
1:A:162:GLN:O	1:A:164:ASN:N	2.44	0.50
1:A:303:PHE:N	1:A:303:PHE:CD2	2.79	0.50
2:E:543:ILE:O	2:E:544:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HB2	1:B:79:GLN:OE1	2.11	0.50
1:B:94:VAL:O	1:B:113:ASP:HA	2.10	0.50
2:E:529:ARG:CA	2:E:597:THR:CG2	2.86	0.50
2:G:484:ILE:HG23	2:G:500:LEU:HG	1.93	0.50
2:H:494:VAL:HG21	2:H:500:LEU:HD11	1.93	0.50
2:F:619:ASP:OD1	2:F:619:ASP:C	2.55	0.50
2:H:541:LYS:CB	2:H:587:GLN:CD	2.77	0.50
1:D:79:GLN:HA	1:D:82:LEU:HB3	1.93	0.50
2:F:551:VAL:HG12	2:F:558:ILE:CD1	2.42	0.50
2:F:578:SER:OG	2:F:579:LYS:N	2.44	0.50
1:C:206:ALA:HB2	1:C:242:PHE:HB2	1.94	0.50
2:G:563:ILE:HG22	2:G:595:LEU:HG	1.91	0.50
1:A:118:LYS:HB3	1:A:119:PRO:CD	2.40	0.50
1:C:81:ARG:HH21	1:C:84:LEU:HD11	1.76	0.50
1:D:171:LYS:NZ	1:D:261:GLU:OE1	2.44	0.50
2:G:494:VAL:HG21	2:G:500:LEU:HD11	1.93	0.50
1:A:61:ASN:O	1:A:63:LYS:N	2.41	0.50
1:B:322:VAL:O	1:B:391:ILE:HA	2.12	0.50
2:F:459:LEU:O	2:F:496:PRO:HA	2.11	0.50
2:H:571:ASP:OD1	2:H:572:LYS:N	2.44	0.50
1:A:97:CYS:SG	1:A:111:ASN:ND2	2.85	0.50
1:A:118:LYS:HB3	1:A:119:PRO:HD2	1.93	0.50
1:B:252:LYS:HG2	1:B:253:LEU:N	2.27	0.50
1:B:277:ASN:O	1:B:280:PHE:N	2.44	0.50
1:B:303:PHE:N	1:B:303:PHE:CD2	2.79	0.50
1:B:310:LYS:HA	1:B:313:GLU:HB2	1.93	0.50
1:D:264:PHE:CZ	1:D:268:ILE:HD11	2.46	0.50
1:D:402:PHE:HZ	1:D:410:GLY:H	1.58	0.50
2:E:445:VAL:HG22	2:E:556:THR:HG21	1.93	0.50
2:G:542:SER:O	2:G:543:ILE:HG12	2.12	0.50
2:H:626:ILE:HG22	2:H:627:GLY:N	2.25	0.50
1:B:44:GLN:O	1:B:47:ARG:HB3	2.12	0.49
1:C:310:LYS:O	1:C:314:MET:HG2	2.11	0.49
1:C:397:GLN:C	1:C:399:GLY:N	2.64	0.49
2:E:450:ASP:CG	2:E:451:MET:N	2.69	0.49
2:E:475:ASN:HB3	2:E:477:HIS:HB2	1.93	0.49
2:F:529:ARG:HA	2:F:597:THR:HG22	1.94	0.49
2:H:467:GLY:H	2:H:481:VAL:HG12	1.76	0.49
2:H:554:ILE:CD1	2:H:601:ILE:HG21	2.41	0.49
2:H:563:ILE:HA	2:H:594:ARG:O	2.12	0.49
1:A:271:SER:O	1:A:272:THR:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:HG22	1:B:38:ILE:O	2.11	0.49
2:E:475:ASN:O	2:E:476:LYS:C	2.54	0.49
1:B:61:ASN:O	1:B:63:LYS:N	2.40	0.49
1:B:97:CYS:SG	1:B:111:ASN:ND2	2.85	0.49
1:B:117:PHE:CZ	1:B:139:LEU:O	2.65	0.49
1:C:252:LYS:HG2	1:C:253:LEU:N	2.27	0.49
2:F:594:ARG:C	2:F:595:LEU:HD12	2.37	0.49
1:A:51:MET:O	1:A:51:MET:HG2	2.13	0.49
1:A:275:LEU:N	1:A:275:LEU:HD12	2.28	0.49
1:C:69:LEU:O	1:C:70:SER:C	2.55	0.49
1:C:151:ILE:CG2	1:C:232:PHE:CG	2.96	0.49
2:F:441:ARG:HB2	2:F:461:SER:HB3	1.94	0.49
2:H:486:SER:HB2	2:H:500:LEU:HD11	1.94	0.49
1:A:40:PRO:HB3	1:A:122:THR:H	1.78	0.49
1:A:286:LEU:CD1	1:A:390:GLU:HG3	2.43	0.49
1:A:310:LYS:HA	1:A:313:GLU:HB2	1.94	0.49
1:B:133:THR:C	1:B:135:ALA:N	2.64	0.49
1:B:276:SER:HA	1:B:279:LYS:CE	2.41	0.49
1:C:226:LEU:HB2	1:C:253:LEU:HD23	1.95	0.49
1:D:226:LEU:HB2	1:D:253:LEU:HD23	1.95	0.49
2:E:520:ASP:O	2:E:524:LEU:HB3	2.13	0.49
1:A:244:GLN:HB3	1:A:245:ARG:HD2	1.93	0.49
2:G:456:LEU:CD2	2:G:501:LYS:CG	2.90	0.49
2:G:467:GLY:H	2:G:481:VAL:HG12	1.77	0.49
2:H:441:ARG:N	2:H:461:SER:O	2.45	0.49
1:B:40:PRO:HB3	1:B:122:THR:H	1.78	0.49
2:H:456:LEU:CD2	2:H:501:LYS:CE	2.86	0.49
1:A:44:GLN:O	1:A:47:ARG:HB3	2.12	0.49
1:B:22:LYS:C	1:B:24:LEU:H	2.20	0.49
1:C:78:VAL:O	1:C:82:LEU:HB2	2.12	0.49
1:D:206:ALA:HB2	1:D:242:PHE:HB2	1.94	0.49
1:D:252:LYS:HG2	1:D:253:LEU:N	2.27	0.49
2:E:441:ARG:HB2	2:E:461:SER:HB3	1.94	0.49
2:F:520:ASP:OD1	2:F:522:ASN:ND2	2.42	0.49
1:B:118:LYS:HB3	1:B:119:PRO:CD	2.41	0.49
1:C:171:LYS:NZ	1:C:261:GLU:OE1	2.45	0.49
2:E:578:SER:OG	2:E:579:LYS:N	2.44	0.49
2:E:609:PHE:HB3	2:E:611:GLN:NE2	2.27	0.49
2:F:467:GLY:O	2:F:480:GLU:HG3	2.13	0.49
2:F:467:GLY:N	2:F:481:VAL:HB	2.28	0.49
2:F:551:VAL:CG1	2:F:558:ILE:HD11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:633:VAL:HA	2:F:634:PRO:HA	1.65	0.49
2:H:554:ILE:HD12	2:H:601:ILE:CG2	2.42	0.49
1:B:41:PRO:O	1:B:42:LYS:CG	2.55	0.49
1:D:78:VAL:O	1:D:82:LEU:HB2	2.13	0.49
2:H:456:LEU:CD2	2:H:501:LYS:CG	2.90	0.49
1:A:52:LEU:HB2	1:A:79:GLN:OE1	2.12	0.48
1:A:314:MET:O	1:A:315:GLY:C	2.55	0.48
1:D:69:LEU:O	1:D:70:SER:C	2.55	0.48
2:E:441:ARG:NE	2:E:525:CYS:SG	2.86	0.48
2:E:594:ARG:C	2:E:595:LEU:HD12	2.37	0.48
2:E:619:ASP:OD1	2:E:619:ASP:C	2.55	0.48
1:B:133:THR:O	1:B:134:GLU:C	2.55	0.48
1:D:233:LYS:O	1:D:237:SER:N	2.44	0.48
2:E:529:ARG:O	2:E:597:THR:HG22	2.13	0.48
2:E:544:ILE:CG2	2:E:563:ILE:HD11	2.43	0.48
2:G:441:ARG:N	2:G:461:SER:O	2.44	0.48
2:G:563:ILE:HA	2:G:594:ARG:O	2.14	0.48
2:H:530:THR:C	2:H:633:VAL:CG2	2.83	0.48
1:A:277:ASN:O	1:A:280:PHE:N	2.46	0.48
1:C:320:LEU:HD23	1:C:389:LEU:HD13	1.96	0.48
1:D:40:PRO:HD3	1:D:123:SER:HB2	1.95	0.48
1:D:317:VAL:HG12	1:D:413:LEU:CD2	2.42	0.48
1:A:252:LYS:HG2	1:A:253:LEU:N	2.29	0.48
1:A:305:VAL:CG2	1:A:306:GLU:N	2.76	0.48
2:F:445:VAL:HG22	2:F:556:THR:HG21	1.94	0.48
2:G:554:ILE:HD12	2:G:601:ILE:CG2	2.42	0.48
1:A:399:GLY:O	1:A:403:VAL:HG23	2.14	0.48
2:E:460:GLU:HB3	2:E:611:GLN:HG3	1.95	0.48
2:E:473:MET:HG2	2:E:602:CYS:HB2	1.94	0.48
2:G:447:LYS:CD	2:G:512:ILE:O	2.62	0.48
1:A:89:PRO:O	1:A:91:ASN:N	2.47	0.48
1:B:52:LEU:HD12	1:B:79:GLN:HG3	1.95	0.48
1:B:318:GLU:HB2	1:B:414:ARG:HG2	1.94	0.48
1:D:203:ARG:O	1:D:207:GLU:HB2	2.14	0.48
1:D:330:ARG:HB2	1:D:374:LEU:HD23	1.96	0.48
2:E:473:MET:HG3	2:E:474:PRO:HA	1.96	0.48
2:E:502:ILE:HB	2:E:504:LEU:CD1	2.44	0.48
2:H:542:SER:O	2:H:543:ILE:HG12	2.13	0.48
1:A:121:ASN:OD1	1:A:121:ASN:O	2.32	0.48
1:B:399:GLY:O	1:B:403:VAL:HG23	2.14	0.48
1:D:8:ALA:C	1:D:10:ARG:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:LEU:C	1:D:124:LEU:HD23	2.39	0.48
1:D:151:ILE:CG2	1:D:232:PHE:CG	2.96	0.48
2:G:486:SER:HB2	2:G:500:LEU:HD11	1.94	0.48
2:H:469:GLN:O	2:H:521:PRO:HG3	2.14	0.48
1:B:81:ARG:CD	1:B:111:ASN:HB3	2.40	0.48
1:B:234:THR:HG22	1:B:234:THR:O	2.13	0.48
2:G:468:GLN:HB3	2:G:470:LEU:HD13	1.95	0.48
2:H:605:THR:O	2:H:606:PHE:C	2.56	0.48
1:A:41:PRO:O	1:A:42:LYS:CG	2.52	0.48
1:A:151:ILE:O	1:A:228:GLY:HA2	2.14	0.48
1:B:271:SER:O	1:B:272:THR:C	2.56	0.48
1:D:317:VAL:HA	1:D:413:LEU:HA	1.95	0.48
2:F:546:PRO:CD	2:F:583:ARG:O	2.62	0.48
2:G:603:LEU:C	2:G:604:GLU:HG2	2.39	0.48
1:A:22:LYS:C	1:A:24:LEU:H	2.22	0.48
1:B:275:LEU:HD12	1:B:275:LEU:N	2.29	0.48
2:F:473:MET:HG3	2:F:474:PRO:HA	1.96	0.48
2:F:529:ARG:CA	2:F:597:THR:CG2	2.92	0.48
2:G:540:HIS:HB3	2:G:541:LYS:C	2.33	0.48
1:B:89:PRO:HB2	1:B:115:GLU:CD	2.39	0.47
1:B:314:MET:O	1:B:315:GLY:C	2.56	0.47
1:C:233:LYS:O	1:C:237:SER:N	2.44	0.47
2:E:467:GLY:O	2:E:480:GLU:HG3	2.14	0.47
2:E:551:VAL:HG12	2:E:558:ILE:CD1	2.44	0.47
2:E:569:LEU:H	2:E:578:SER:CB	2.27	0.47
2:F:502:ILE:HB	2:F:504:LEU:CD1	2.44	0.47
2:F:609:PHE:HB3	2:F:611:GLN:NE2	2.29	0.47
2:H:520:ASP:OD1	2:H:522:ASN:ND2	2.37	0.47
2:E:540:HIS:HA	2:E:624:ILE:HG13	1.95	0.47
2:H:633:VAL:O	2:H:634:PRO:C	2.57	0.47
1:B:91:ASN:C	1:B:120:ILE:HG22	2.21	0.47
1:C:239:SER:C	1:C:241:MET:H	2.22	0.47
1:D:320:LEU:HD23	1:D:389:LEU:HD13	1.97	0.47
2:E:467:GLY:N	2:E:481:VAL:HB	2.29	0.47
1:B:51:MET:O	1:B:51:MET:HG2	2.13	0.47
1:B:286:LEU:CD1	1:B:390:GLU:HG3	2.43	0.47
1:C:124:LEU:HD23	1:C:124:LEU:C	2.38	0.47
1:C:319:ILE:HD12	1:C:412:ILE:HD12	1.97	0.47
1:C:330:ARG:HB2	1:C:374:LEU:HD23	1.96	0.47
2:G:619:ASP:C	2:G:619:ASP:OD1	2.57	0.47
1:A:234:THR:O	1:A:234:THR:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASN:OD1	1:B:121:ASN:O	2.33	0.47
1:B:146:PHE:O	1:B:160:THR:HA	2.14	0.47
1:B:303:PHE:HD2	1:B:303:PHE:H	1.63	0.47
2:G:450:ASP:CG	2:G:451:MET:N	2.69	0.47
2:H:447:LYS:CD	2:H:512:ILE:O	2.61	0.47
2:G:456:LEU:CD2	2:G:501:LYS:CE	2.85	0.47
2:G:633:VAL:O	2:G:634:PRO:C	2.57	0.47
2:H:619:ASP:OD1	2:H:619:ASP:C	2.56	0.47
1:A:133:THR:O	1:A:134:GLU:C	2.57	0.47
1:B:14:ILE:HG23	1:B:140:LEU:HD22	1.95	0.47
1:C:151:ILE:HG22	1:C:232:PHE:CD2	2.50	0.47
1:C:317:VAL:HA	1:C:413:LEU:HA	1.96	0.47
1:C:318:GLU:HB2	1:C:414:ARG:HH21	1.79	0.47
1:D:323:TYR:HE2	1:D:394:ASP:HB3	1.80	0.47
2:E:569:LEU:H	2:E:578:SER:HB3	1.79	0.47
2:F:540:HIS:HA	2:F:624:ILE:HG13	1.96	0.47
2:F:543:ILE:O	2:F:544:ILE:HG13	2.13	0.47
2:G:546:PRO:CD	2:G:583:ARG:O	2.57	0.47
2:H:495:ALA:HB1	2:H:496:PRO:CD	2.39	0.47
1:A:176:LEU:HA	1:A:197:LYS:HD2	1.96	0.47
1:A:322:VAL:HG12	1:A:323:TYR:N	2.29	0.47
1:B:275:LEU:H	1:B:275:LEU:CD1	2.28	0.47
1:C:203:ARG:O	1:C:207:GLU:HB2	2.14	0.47
2:E:537:ILE:O	2:E:588:ASP:N	2.44	0.47
2:F:473:MET:HB3	2:F:474:PRO:CD	2.39	0.47
2:G:469:GLN:O	2:G:521:PRO:HG3	2.15	0.47
1:A:62:ILE:HG21	1:A:68:ARG:HB2	1.95	0.47
1:B:305:VAL:CG2	1:B:306:GLU:N	2.77	0.47
2:E:473:MET:CB	2:E:474:PRO:CD	2.93	0.47
2:G:569:LEU:H	2:G:578:SER:CB	2.28	0.47
2:H:540:HIS:CE1	2:H:624:ILE:HD11	2.49	0.47
1:A:303:PHE:HD2	1:A:303:PHE:H	1.62	0.47
1:B:118:LYS:CE	1:B:119:PRO:CG	2.79	0.47
1:B:124:LEU:C	1:B:124:LEU:CD2	2.87	0.47
1:C:402:PHE:HZ	1:C:410:GLY:H	1.62	0.47
2:E:528:GLY:O	2:E:600:THR:HG23	2.14	0.47
2:F:544:ILE:CG2	2:F:563:ILE:HD11	2.45	0.47
2:H:540:HIS:HB3	2:H:541:LYS:C	2.33	0.47
1:C:8:ALA:C	1:C:10:ARG:H	2.22	0.46
2:E:500:LEU:C	2:E:501:LYS:HG3	2.41	0.46
2:G:520:ASP:OD1	2:G:522:ASN:ND2	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:540:HIS:CE1	2:G:624:ILE:HD11	2.50	0.46
1:C:40:PRO:HD3	1:C:123:SER:HB2	1.97	0.46
1:D:151:ILE:HG22	1:D:232:PHE:CD2	2.51	0.46
1:D:239:SER:C	1:D:241:MET:H	2.23	0.46
2:F:529:ARG:CA	2:F:597:THR:HG22	2.45	0.46
2:G:609:PHE:HB3	2:G:611:GLN:HE22	1.80	0.46
2:H:609:PHE:HB3	2:H:611:GLN:HE22	1.81	0.46
1:A:124:LEU:C	1:A:124:LEU:CD2	2.88	0.46
2:E:544:ILE:HG12	2:E:548:TYR:CG	2.50	0.46
1:A:271:SER:O	1:A:273:GLU:N	2.48	0.46
1:A:399:GLY:O	1:A:400:SER:C	2.59	0.46
1:B:68:ARG:O	1:B:70:SER:N	2.48	0.46
1:A:146:PHE:O	1:A:160:THR:HA	2.15	0.46
1:B:151:ILE:CG2	1:B:232:PHE:HB3	2.45	0.46
1:C:214:ILE:HD12	1:C:245:ARG:HD3	1.98	0.46
2:E:529:ARG:HB2	2:E:597:THR:HG23	1.97	0.46
2:F:569:LEU:H	2:F:578:SER:CB	2.29	0.46
2:G:473:MET:HB3	2:G:474:PRO:HA	1.96	0.46
1:A:176:LEU:O	1:A:177:PRO:C	2.58	0.46
1:B:89:PRO:O	1:B:91:ASN:N	2.49	0.46
1:B:117:PHE:CD1	1:B:139:LEU:HD13	2.51	0.46
2:E:551:VAL:CG1	2:E:558:ILE:HD11	2.46	0.46
2:G:446:ASP:HB3	2:G:456:LEU:HD13	1.98	0.46
2:G:612:MET:HE3	2:G:612:MET:HB3	1.68	0.46
2:H:569:LEU:H	2:H:578:SER:CB	2.29	0.46
1:A:276:SER:HA	1:A:279:LYS:CE	2.43	0.46
1:B:302:CYS:HB3	1:B:413:LEU:HD11	1.98	0.46
1:C:413:LEU:HD13	1:C:417:VAL:HG23	1.97	0.46
1:D:214:ILE:HD12	1:D:245:ARG:HD3	1.98	0.46
1:D:319:ILE:HD12	1:D:412:ILE:HD12	1.98	0.46
2:F:474:PRO:HG3	2:F:602:CYS:HB3	1.98	0.46
2:F:529:ARG:HB2	2:F:597:THR:CG2	2.46	0.46
1:B:176:LEU:HA	1:B:197:LYS:HD2	1.97	0.46
2:E:540:HIS:CB	2:E:541:LYS:CA	2.36	0.46
2:F:604:GLU:HB2	2:F:612:MET:HB2	1.98	0.46
2:G:453:THR:OG1	2:G:509:GLU:HB3	2.16	0.46
1:A:275:LEU:CD1	1:A:275:LEU:H	2.29	0.46
1:B:151:ILE:O	1:B:228:GLY:HA2	2.16	0.46
1:B:347:THR:CB	1:B:348:PRO:CD	2.70	0.46
2:E:620:GLU:HB3	2:E:621:GLY:H	1.48	0.46
2:H:453:THR:OG1	2:H:509:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ILE:HG21	1:B:68:ARG:HB2	1.97	0.45
1:B:93:LEU:HA	1:B:93:LEU:HD23	1.48	0.45
1:D:79:GLN:HG2	1:D:82:LEU:HD23	1.98	0.45
1:D:294:ILE:C	1:D:296:GLN:N	2.71	0.45
2:G:442:LEU:HD12	2:G:458:LYS:O	2.16	0.45
2:G:520:ASP:O	2:G:524:LEU:HB3	2.16	0.45
2:G:603:LEU:O	2:G:604:GLU:CG	2.59	0.45
2:G:609:PHE:HB3	2:G:611:GLN:NE2	2.31	0.45
1:A:300:LYS:H	1:A:300:LYS:HD2	1.80	0.45
1:B:176:LEU:O	1:B:177:PRO:C	2.59	0.45
1:C:303:PHE:HE1	2:G:583:ARG:HE	1.62	0.45
2:E:515:GLY:HA2	2:E:557:CYS:N	2.30	0.45
2:E:633:VAL:HA	2:E:634:PRO:HA	1.67	0.45
1:A:61:ASN:C	1:A:63:LYS:H	2.24	0.45
1:B:61:ASN:C	1:B:63:LYS:H	2.24	0.45
1:B:397:GLN:NE2	2:E:549:ASN:H	2.14	0.45
1:C:71:VAL:C	1:C:73:GLY:H	2.24	0.45
1:C:416:ARG:HE	1:C:417:VAL:C	2.24	0.45
1:D:268:ILE:HG22	1:D:268:ILE:O	2.17	0.45
2:E:552:LEU:HD21	2:E:554:ILE:HD11	1.97	0.45
2:G:486:SER:HB2	2:G:500:LEU:CD1	2.46	0.45
1:A:318:GLU:HB2	1:A:414:ARG:HG2	1.99	0.45
1:A:347:THR:CB	1:A:348:PRO:CD	2.68	0.45
1:C:197:LYS:HA	1:C:200:ASN:HB2	1.97	0.45
2:H:605:THR:HA	2:H:629:VAL:HG13	1.97	0.45
2:E:444:ILE:HD12	2:E:516:PHE:HB2	1.98	0.45
2:H:474:PRO:HD2	2:H:516:PHE:CD1	2.52	0.45
1:B:91:ASN:CB	1:B:118:LYS:O	2.64	0.45
1:B:275:LEU:C	1:B:277:ASN:N	2.59	0.45
1:C:79:GLN:HG2	1:C:82:LEU:HD23	1.97	0.45
1:C:166:ARG:HE	1:C:166:ARG:N	2.12	0.45
2:E:538:ILE:HG12	2:E:625:ALA:HA	1.99	0.45
2:E:558:ILE:O	2:E:558:ILE:HG13	2.17	0.45
2:E:619:ASP:OD1	2:E:620:GLU:N	2.50	0.45
2:F:445:VAL:HG22	2:F:556:THR:HG22	1.99	0.45
2:F:479:VAL:CG2	2:F:504:LEU:HD23	2.32	0.45
2:F:619:ASP:OD1	2:F:620:GLU:N	2.50	0.45
2:H:486:SER:HB2	2:H:500:LEU:CD1	2.46	0.45
1:A:52:LEU:HD12	1:A:79:GLN:HG3	1.99	0.45
1:A:87:LYS:HD3	1:A:88:VAL:H	1.82	0.45
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ILE:O	1:C:268:ILE:HG22	2.17	0.45
1:C:327:ASP:HB3	1:C:348:PRO:HD3	1.99	0.45
2:E:536:VAL:HG21	2:H:488:ASP:HB2	1.98	0.45
2:F:500:LEU:C	2:F:501:LYS:HG3	2.42	0.45
2:H:473:MET:HB3	2:H:474:PRO:HA	1.97	0.45
2:H:620:GLU:HB3	2:H:621:GLY:H	1.47	0.45
1:A:81:ARG:CD	1:A:111:ASN:HB3	2.41	0.45
1:A:118:LYS:CE	1:A:119:PRO:HG3	2.39	0.45
1:A:305:VAL:O	1:A:306:GLU:C	2.59	0.45
2:G:629:VAL:HG13	2:G:629:VAL:O	2.17	0.45
2:H:442:LEU:HD12	2:H:458:LYS:O	2.17	0.45
1:A:45:ILE:HG13	1:A:88:VAL:HG22	1.97	0.45
1:A:294:ILE:C	1:A:296:GLN:H	2.25	0.45
1:A:397:GLN:NE2	2:F:549:ASN:H	2.15	0.45
1:B:45:ILE:HG13	1:B:88:VAL:HG22	1.99	0.45
1:B:91:ASN:CB	1:B:119:PRO:HA	2.46	0.45
1:B:124:LEU:C	1:B:124:LEU:HD23	2.41	0.45
1:C:301:TYR:H	1:C:301:TYR:HD2	1.65	0.45
1:D:71:VAL:C	1:D:73:GLY:H	2.24	0.45
1:D:152:ASP:CG	1:D:259:GLY:HA3	2.42	0.45
2:F:569:LEU:H	2:F:578:SER:HB3	1.81	0.45
2:H:520:ASP:O	2:H:524:LEU:HB3	2.16	0.45
2:H:603:LEU:C	2:H:604:GLU:HG2	2.39	0.45
1:B:223:GLY:HA2	1:B:251:LEU:HD22	1.98	0.45
1:C:147:GLY:HA3	1:C:224:LEU:HD22	1.99	0.45
2:E:447:LYS:HD2	2:E:512:ILE:O	2.17	0.45
2:F:515:GLY:HA2	2:F:557:CYS:N	2.32	0.45
2:F:517:ILE:HD11	2:F:602:CYS:HB2	1.99	0.45
1:A:89:PRO:HB2	1:A:115:GLU:CD	2.41	0.44
1:A:151:ILE:CG2	1:A:232:PHE:HB3	2.46	0.44
1:B:275:LEU:HD12	1:B:275:LEU:H	1.82	0.44
1:C:226:LEU:HD12	1:C:253:LEU:HD21	2.00	0.44
1:D:327:ASP:HB3	1:D:348:PRO:HD3	1.99	0.44
1:D:329:MET:HB3	1:D:331:TYR:HE1	1.82	0.44
2:E:535:ILE:HG22	2:E:536:VAL:N	2.31	0.44
2:H:446:ASP:HB3	2:H:456:LEU:HD13	1.99	0.44
2:H:609:PHE:HB3	2:H:611:GLN:NE2	2.32	0.44
1:A:124:LEU:C	1:A:124:LEU:HD23	2.42	0.44
1:A:326:LEU:CD2	1:A:328:ILE:HD12	2.47	0.44
1:D:166:ARG:HE	1:D:166:ARG:N	2.13	0.44
2:G:605:THR:HA	2:G:629:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:535:ILE:HG22	2:F:536:VAL:N	2.33	0.44
2:F:612:MET:HE3	2:F:612:MET:HB3	1.66	0.44
2:G:442:LEU:HD12	2:G:458:LYS:C	2.42	0.44
2:H:442:LEU:HD12	2:H:458:LYS:C	2.42	0.44
1:B:287:ILE:HD13	1:B:402:PHE:HB2	1.98	0.44
1:D:8:ALA:C	1:D:10:ARG:N	2.73	0.44
1:D:214:ILE:HA	1:D:219:VAL:HA	1.99	0.44
2:F:552:LEU:HD21	2:F:554:ILE:HD11	1.99	0.44
2:F:555:HIS:N	2:F:557:CYS:SG	2.90	0.44
2:H:450:ASP:CG	2:H:451:MET:N	2.70	0.44
1:A:223:GLY:HA2	1:A:251:LEU:HD22	2.00	0.44
1:A:270:LEU:HD13	1:A:270:LEU:HA	1.87	0.44
1:A:328:ILE:HG22	1:A:345:TYR:HB3	2.00	0.44
1:B:305:VAL:O	1:B:306:GLU:C	2.59	0.44
2:F:529:ARG:O	2:F:597:THR:HG22	2.17	0.44
2:G:540:HIS:HB2	2:G:587:GLN:HG3	2.00	0.44
1:A:58:THR:C	1:A:60:SER:N	2.76	0.44
1:C:8:ALA:C	1:C:10:ARG:N	2.73	0.44
1:D:234:THR:HG22	1:D:234:THR:O	2.18	0.44
2:E:612:MET:HB3	2:E:612:MET:HE3	1.63	0.44
1:B:87:LYS:HD3	1:B:88:VAL:H	1.82	0.44
1:D:197:LYS:HA	1:D:200:ASN:HB2	1.99	0.44
2:G:619:ASP:OD1	2:G:620:GLU:N	2.51	0.44
1:A:287:ILE:HD13	1:A:402:PHE:HB2	1.98	0.44
1:A:380:ASN:O	1:A:381:ASN:HB3	2.17	0.44
1:B:233:LYS:O	1:B:237:SER:CB	2.66	0.44
1:B:271:SER:O	1:B:273:GLU:N	2.51	0.44
1:B:293:GLU:O	1:B:296:GLN:N	2.49	0.44
2:E:447:LYS:O	2:E:448:TYR:CB	2.55	0.44
2:E:555:HIS:N	2:E:557:CYS:SG	2.91	0.44
2:E:604:GLU:HB2	2:E:612:MET:HB2	2.00	0.44
2:F:502:ILE:H	2:F:502:ILE:HG12	1.65	0.44
2:G:474:PRO:HD2	2:G:516:PHE:CD1	2.52	0.44
2:G:566:LEU:CD1	2:G:582:PRO:O	2.65	0.44
2:H:612:MET:HB3	2:H:612:MET:HE3	1.69	0.44
1:A:121:ASN:O	1:A:122:THR:CB	2.65	0.44
1:B:22:LYS:O	1:B:24:LEU:N	2.51	0.44
1:B:151:ILE:CD1	1:B:205:VAL:HG11	2.48	0.44
1:D:147:GLY:HA3	1:D:224:LEU:HD22	2.00	0.44
2:E:575:GLY:HA2	2:H:489:VAL:HG11	1.99	0.44
1:B:326:LEU:CD2	1:B:328:ILE:HD12	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ILE:HB	1:C:412:ILE:HB	2.00	0.43
2:F:447:LYS:HD2	2:F:512:ILE:O	2.18	0.43
2:F:487:ASP:HB3	2:F:488:ASP:H	1.73	0.43
1:A:68:ARG:O	1:A:70:SER:N	2.51	0.43
1:A:233:LYS:O	1:A:237:SER:CB	2.66	0.43
1:A:275:LEU:HD12	1:A:275:LEU:H	1.84	0.43
1:D:94:VAL:O	1:D:113:ASP:HA	2.18	0.43
1:D:301:TYR:H	1:D:301:TYR:HD2	1.65	0.43
2:E:533:ALA:O	2:E:592:ILE:HA	2.18	0.43
2:H:552:LEU:HD11	2:H:554:ILE:HG12	2.00	0.43
1:A:110:VAL:CG2	1:A:112:ILE:CD1	2.96	0.43
1:B:399:GLY:O	1:B:400:SER:C	2.60	0.43
1:C:234:THR:O	1:C:234:THR:HG22	2.18	0.43
1:C:329:MET:HB3	1:C:331:TYR:HE1	1.82	0.43
2:F:561:VAL:CG2	2:F:596:ARG:O	2.65	0.43
2:H:443:PRO:HD2	2:H:458:LYS:O	2.19	0.43
1:A:91:ASN:CB	1:A:119:PRO:HA	2.46	0.43
1:A:133:THR:C	1:A:135:ALA:H	2.27	0.43
1:A:293:GLU:O	1:A:296:GLN:N	2.51	0.43
1:B:206:ALA:HB2	1:B:242:PHE:HB2	2.00	0.43
1:C:294:ILE:C	1:C:296:GLN:N	2.72	0.43
1:D:151:ILE:HG21	1:D:232:PHE:HB3	1.98	0.43
2:G:541:LYS:CD	2:G:587:GLN:NE2	2.64	0.43
1:A:91:ASN:CB	1:A:118:LYS:O	2.64	0.43
1:A:156:ALA:HB2	1:A:201:TYR:OH	2.19	0.43
3:A:1526:ATP:O2G	3:A:1526:ATP:H5'1	2.18	0.43
1:B:110:VAL:CG2	1:B:112:ILE:CD1	2.97	0.43
1:B:121:ASN:O	1:B:122:THR:CB	2.65	0.43
1:B:156:ALA:HB2	1:B:201:TYR:OH	2.19	0.43
1:D:329:MET:HB3	1:D:331:TYR:CE1	2.53	0.43
2:F:577:LYS:HB3	2:F:577:LYS:HE2	1.87	0.43
2:G:486:SER:CA	2:G:500:LEU:HD12	2.47	0.43
1:A:22:LYS:C	1:A:22:LYS:HD2	2.43	0.43
1:A:43:ASP:CG	1:A:44:GLN:H	2.25	0.43
1:B:118:LYS:HG3	1:B:119:PRO:CD	2.28	0.43
1:B:347:THR:C	1:B:349:GLU:N	2.77	0.43
1:B:380:ASN:O	1:B:381:ASN:HB3	2.19	0.43
1:C:292:ASP:C	1:C:294:ILE:H	2.26	0.43
2:E:517:ILE:HD11	2:E:602:CYS:HB2	2.00	0.43
2:E:524:LEU:CD1	2:E:525:CYS:H	2.32	0.43
2:F:517:ILE:HG12	2:F:602:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:536:VAL:HG21	2:G:488:ASP:HB2	1.99	0.43
2:F:575:GLY:HA2	2:G:489:VAL:HG11	2.01	0.43
1:A:151:ILE:CD1	1:A:205:VAL:HG11	2.49	0.43
1:B:24:LEU:HD23	1:B:24:LEU:HA	1.77	0.43
1:B:270:LEU:HD13	1:B:270:LEU:HA	1.86	0.43
1:C:221:VAL:HB	1:C:222:ALA:H	1.61	0.43
2:G:552:LEU:HD11	2:G:554:ILE:HG12	2.01	0.43
2:H:566:LEU:CD1	2:H:582:PRO:O	2.67	0.43
1:B:85:TYR:CZ	1:B:93:LEU:HD21	2.53	0.43
1:D:221:VAL:HB	1:D:222:ALA:H	1.60	0.43
1:D:231:ASP:O	1:D:235:GLU:HB2	2.18	0.43
2:E:467:GLY:O	2:E:468:GLN:C	2.60	0.43
2:G:567:ILE:HB	2:G:568:CYS:H	1.71	0.43
2:H:619:ASP:OD1	2:H:620:GLU:N	2.51	0.43
2:H:629:VAL:HG13	2:H:629:VAL:O	2.18	0.43
1:A:74:ALA:O	1:A:78:VAL:HG12	2.19	0.43
1:A:206:ALA:HB2	1:A:242:PHE:HB2	1.99	0.43
1:B:118:LYS:HD2	1:B:118:LYS:HA	1.51	0.43
1:C:152:ASP:CG	1:C:259:GLY:HA3	2.44	0.43
1:C:308:THR:O	1:C:312:LEU:N	2.43	0.43
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.79	0.43
1:C:329:MET:HB3	1:C:331:TYR:CE1	2.53	0.43
1:D:302:CYS:HB2	1:D:307:ASP:HB3	2.01	0.43
1:D:309:LEU:O	1:D:313:GLU:HG2	2.19	0.43
1:A:64:SER:O	1:A:65:ARG:C	2.61	0.43
1:A:233:LYS:C	1:A:235:GLU:N	2.76	0.43
1:B:420:GLN:H	1:B:420:GLN:NE2	2.17	0.43
2:F:444:ILE:HG12	2:F:455:VAL:HG11	2.00	0.43
1:B:244:GLN:HE21	1:B:244:GLN:HB2	1.51	0.42
1:D:317:VAL:O	1:D:318:GLU:C	2.62	0.42
2:E:444:ILE:HG12	2:E:455:VAL:HG11	2.01	0.42
2:E:445:VAL:HG22	2:E:556:THR:HG22	1.99	0.42
2:E:487:ASP:HB3	2:E:488:ASP:H	1.74	0.42
2:F:524:LEU:CD1	2:F:525:CYS:H	2.26	0.42
2:F:533:ALA:O	2:F:592:ILE:HA	2.19	0.42
2:H:540:HIS:CE1	2:H:543:ILE:O	2.71	0.42
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.74	0.42
1:A:258:TYR:CD1	1:A:266:GLN:NE2	2.87	0.42
1:B:64:SER:O	1:B:65:ARG:C	2.62	0.42
2:G:486:SER:O	2:G:488:ASP:N	2.52	0.42
1:A:117:PHE:CD1	1:A:139:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ILE:C	1:B:296:GLN:H	2.26	0.42
1:C:71:VAL:C	1:C:73:GLY:N	2.77	0.42
1:C:302:CYS:HB2	1:C:307:ASP:HB3	2.02	0.42
2:E:486:SER:O	2:E:488:ASP:N	2.53	0.42
2:E:545:CYS:CB	2:E:546:PRO:CD	2.75	0.42
2:E:546:PRO:CD	2:E:583:ARG:O	2.64	0.42
2:H:561:VAL:HG23	2:H:596:ARG:O	2.20	0.42
1:A:88:VAL:HA	1:A:89:PRO:HD2	1.74	0.42
1:A:405:GLY:O	2:F:583:ARG:HB3	2.20	0.42
1:C:382:TYR:CD1	1:C:389:LEU:HB2	2.54	0.42
2:E:464:ILE:CG2	2:E:494:VAL:HG13	2.48	0.42
2:F:464:ILE:CG2	2:F:494:VAL:HG13	2.47	0.42
2:F:534:GLN:HB2	2:F:630:LEU:HD11	2.02	0.42
2:F:543:ILE:HG22	2:F:544:ILE:CA	2.50	0.42
2:H:563:ILE:CG2	2:H:595:LEU:HG	2.50	0.42
1:A:68:ARG:C	1:A:70:SER:N	2.78	0.42
1:B:68:ARG:C	1:B:70:SER:N	2.76	0.42
1:B:258:TYR:CD1	1:B:266:GLN:NE2	2.88	0.42
1:B:328:ILE:HG22	1:B:345:TYR:HB3	2.02	0.42
1:C:317:VAL:O	1:C:318:GLU:C	2.63	0.42
1:C:347:THR:OG1	1:C:349:GLU:OE1	2.36	0.42
1:D:71:VAL:C	1:D:73:GLY:N	2.77	0.42
1:D:226:LEU:HD12	1:D:253:LEU:HD21	2.01	0.42
2:E:468:GLN:O	2:E:469:GLN:C	2.62	0.42
2:E:605:THR:OG1	2:E:608:ASP:HB2	2.20	0.42
2:F:468:GLN:O	2:F:469:GLN:C	2.61	0.42
2:G:540:HIS:CE1	2:G:543:ILE:O	2.72	0.42
2:H:474:PRO:HD2	2:H:516:PHE:CE1	2.55	0.42
1:A:28:ARG:HG3	1:A:130:LYS:HB3	2.01	0.42
1:A:85:TYR:CZ	1:A:93:LEU:HD21	2.54	0.42
1:A:243:ASP:O	1:A:244:GLN:HB2	2.19	0.42
1:B:43:ASP:CG	1:B:44:GLN:H	2.27	0.42
1:B:74:ALA:O	1:B:78:VAL:HG12	2.19	0.42
1:B:420:GLN:O	1:B:420:GLN:HG2	2.18	0.42
2:G:447:LYS:CG	2:G:512:ILE:HG23	2.48	0.42
2:G:529:ARG:HG2	2:G:530:THR:OG1	2.20	0.42
2:H:447:LYS:HD3	2:H:512:ILE:O	2.19	0.42
1:C:279:LYS:O	1:C:283:GLU:HB2	2.20	0.42
1:D:233:LYS:C	1:D:235:GLU:N	2.77	0.42
1:D:251:LEU:HD21	1:D:278:VAL:HG22	2.02	0.42
1:D:413:LEU:H	1:D:413:LEU:HG	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:467:GLY:O	2:F:468:GLN:C	2.62	0.42
2:F:537:ILE:O	2:F:588:ASP:N	2.47	0.42
2:G:470:LEU:HG	2:G:519:CYS:O	2.20	0.42
2:H:603:LEU:O	2:H:604:GLU:CG	2.59	0.42
1:C:251:LEU:HD21	1:C:278:VAL:HG22	2.01	0.42
1:C:283:GLU:CD	1:C:393:THR:H	2.27	0.42
1:D:278:VAL:O	1:D:279:LYS:C	2.63	0.42
1:D:347:THR:OG1	1:D:349:GLU:OE1	2.37	0.42
2:E:543:ILE:HG22	2:E:544:ILE:CA	2.50	0.42
2:F:473:MET:CB	2:F:474:PRO:CD	2.96	0.42
2:G:548:TYR:OH	2:G:624:ILE:HG21	2.20	0.42
2:H:486:SER:O	2:H:488:ASP:N	2.52	0.42
2:H:578:SER:OG	2:H:579:LYS:N	2.41	0.42
1:A:267:ALA:O	1:A:271:SER:HB3	2.20	0.42
1:C:231:ASP:O	1:C:235:GLU:HB2	2.20	0.42
2:E:540:HIS:ND1	2:E:624:ILE:HD11	2.34	0.42
1:A:206:ALA:CB	1:A:242:PHE:HB2	2.50	0.42
1:A:323:TYR:CD1	1:A:325:ASN:O	2.73	0.42
1:A:329:MET:HE2	1:A:329:MET:HB2	1.82	0.42
2:E:520:ASP:OD1	2:E:521:PRO:HD2	2.20	0.42
2:F:454:VAL:CG1	2:F:455:VAL:N	2.83	0.42
1:A:64:SER:O	1:A:67:ASN:N	2.48	0.41
1:A:152:ASP:HB3	1:A:155:GLY:O	2.20	0.41
1:C:213:PHE:CD2	1:C:221:VAL:HG11	2.55	0.41
1:D:283:GLU:CD	1:D:393:THR:H	2.27	0.41
2:F:537:ILE:HD13	2:F:537:ILE:HA	1.83	0.41
2:G:568:CYS:O	2:G:592:ILE:HG12	2.20	0.41
2:G:595:LEU:HD12	2:G:595:LEU:N	2.34	0.41
1:A:103:GLU:C	1:A:105:GLY:H	2.27	0.41
1:A:264:PHE:O	1:A:268:ILE:HG13	2.21	0.41
1:A:347:THR:C	1:A:349:GLU:H	2.25	0.41
1:B:22:LYS:C	1:B:22:LYS:HD2	2.45	0.41
1:B:133:THR:C	1:B:135:ALA:H	2.28	0.41
1:B:294:ILE:HG23	1:B:301:TYR:CZ	2.55	0.41
1:B:322:VAL:CG1	1:B:323:TYR:N	2.83	0.41
1:C:413:LEU:HD13	1:C:417:VAL:CG2	2.50	0.41
1:D:292:ASP:C	1:D:294:ILE:H	2.26	0.41
2:E:534:GLN:HB2	2:E:630:LEU:HD11	2.03	0.41
2:G:474:PRO:O	2:G:475:ASN:C	2.63	0.41
2:H:455:VAL:CG2	2:H:512:ILE:CD1	2.99	0.41
2:H:617:LEU:HD12	2:H:617:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLY:O	1:A:77:SER:HB2	2.19	0.41
1:A:223:GLY:O	1:A:224:LEU:HB2	2.20	0.41
1:C:278:VAL:O	1:C:279:LYS:C	2.63	0.41
1:D:319:ILE:HB	1:D:412:ILE:HB	2.02	0.41
2:F:555:HIS:CD2	2:F:555:HIS:H	2.37	0.41
1:B:121:ASN:O	1:B:122:THR:HG22	2.20	0.41
1:B:139:LEU:HD23	1:B:139:LEU:HA	1.76	0.41
1:B:223:GLY:O	1:B:224:LEU:HB2	2.19	0.41
1:C:166:ARG:HD2	1:C:166:ARG:C	2.46	0.41
1:D:78:VAL:O	1:D:82:LEU:CB	2.69	0.41
2:G:517:ILE:CG1	2:G:602:CYS:SG	3.08	0.41
2:H:608:ASP:O	2:H:609:PHE:C	2.63	0.41
1:A:24:LEU:HA	1:A:24:LEU:HD23	1.75	0.41
1:A:191:ALA:O	1:A:195:MET:N	2.46	0.41
1:A:347:THR:C	1:A:349:GLU:N	2.78	0.41
1:B:103:GLU:C	1:B:105:GLY:H	2.28	0.41
1:B:264:PHE:O	1:B:268:ILE:HG13	2.21	0.41
1:B:329:MET:HB2	1:B:329:MET:HE2	1.84	0.41
1:D:38:ILE:CD1	1:D:135:ALA:CB	2.99	0.41
2:F:544:ILE:HG12	2:F:548:TYR:CG	2.55	0.41
2:G:447:LYS:HD3	2:G:512:ILE:O	2.21	0.41
1:A:121:ASN:O	1:A:122:THR:HG22	2.21	0.41
1:A:167:GLU:HG3	1:B:66:VAL:HG21	2.02	0.41
1:B:73:GLY:O	1:B:77:SER:HB2	2.20	0.41
1:B:115:GLU:CG	1:B:116:PRO:N	2.83	0.41
1:B:294:ILE:HG12	1:B:301:TYR:CD1	2.55	0.41
1:C:94:VAL:O	1:C:113:ASP:HA	2.19	0.41
1:C:214:ILE:HA	1:C:219:VAL:HA	2.01	0.41
1:C:309:LEU:O	1:C:313:GLU:HG2	2.21	0.41
1:D:382:TYR:CD1	1:D:389:LEU:HB2	2.55	0.41
2:E:555:HIS:CD2	2:E:555:HIS:H	2.36	0.41
2:G:471:VAL:HG13	2:G:477:HIS:H	1.84	0.41
2:H:542:SER:C	2:H:543:ILE:HG12	2.45	0.41
1:A:374:LEU:HD23	1:A:374:LEU:HA	1.87	0.41
1:B:78:VAL:O	1:B:79:GLN:C	2.64	0.41
1:B:82:LEU:HD12	1:B:82:LEU:HA	1.95	0.41
1:B:178:LYS:HG3	1:B:178:LYS:H	1.65	0.41
1:B:266:GLN:O	1:B:270:LEU:HD23	2.20	0.41
1:D:213:PHE:CD2	1:D:221:VAL:HG11	2.56	0.41
1:D:236:LEU:O	1:D:242:PHE:HD2	2.04	0.41
1:D:308:THR:O	1:D:312:LEU:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:467:GLY:HA2	2:F:481:VAL:O	2.21	0.41
2:H:470:LEU:HG	2:H:519:CYS:O	2.21	0.41
2:H:486:SER:CA	2:H:500:LEU:HD12	2.46	0.41
2:H:568:CYS:O	2:H:592:ILE:HG12	2.21	0.41
1:A:102:THR:HG23	1:A:103:GLU:N	2.36	0.41
1:B:245:ARG:H	1:B:245:ARG:CD	2.18	0.41
1:D:409:ILE:O	1:D:409:ILE:HG23	2.21	0.41
2:G:474:PRO:HD2	2:G:516:PHE:CE1	2.56	0.41
2:G:486:SER:HG	2:G:498:GLU:CD	2.28	0.41
2:H:567:ILE:HB	2:H:568:CYS:H	1.71	0.41
1:A:224:LEU:O	1:A:250:VAL:HA	2.20	0.41
1:A:233:LYS:O	1:A:237:SER:HB2	2.20	0.41
1:A:266:GLN:O	1:A:270:LEU:HD23	2.20	0.41
1:A:377:TRP:CZ3	1:A:385:PHE:HE2	2.39	0.41
1:A:401:GLN:HB3	2:F:545:CYS:SG	2.61	0.41
1:B:58:THR:C	1:B:60:SER:N	2.75	0.41
1:B:233:LYS:O	1:B:237:SER:HB2	2.21	0.41
1:B:233:LYS:C	1:B:235:GLU:N	2.77	0.41
1:B:243:ASP:O	1:B:244:GLN:HB2	2.20	0.41
1:C:38:ILE:CD1	1:C:135:ALA:CB	2.98	0.41
1:C:136:LEU:C	1:C:138:ALA:H	2.28	0.41
1:C:329:MET:O	1:C:345:TYR:HA	2.21	0.41
1:D:303:PHE:HE1	2:H:583:ARG:HE	1.63	0.41
1:D:329:MET:O	1:D:345:TYR:HA	2.20	0.41
2:E:473:MET:CG	2:E:474:PRO:HD3	2.50	0.41
2:E:517:ILE:HG12	2:E:602:CYS:SG	2.61	0.41
2:F:464:ILE:HD12	2:F:470:LEU:HD21	2.03	0.41
2:G:444:ILE:HD12	2:G:516:PHE:HB2	2.03	0.41
2:G:561:VAL:HG11	2:G:617:LEU:HD11	2.03	0.41
2:G:570:VAL:HG12	2:G:591:CYS:HA	2.03	0.41
2:H:447:LYS:CG	2:H:512:ILE:HG23	2.49	0.41
2:H:595:LEU:HD12	2:H:595:LEU:N	2.35	0.41
1:B:206:ALA:CB	1:B:242:PHE:HB2	2.50	0.41
1:C:204:LYS:HA	1:C:207:GLU:HB3	2.03	0.41
1:C:233:LYS:C	1:C:235:GLU:N	2.78	0.41
2:F:444:ILE:HD12	2:F:516:PHE:HB2	2.03	0.41
2:G:543:ILE:HG22	2:G:544:ILE:CA	2.51	0.41
2:G:606:PHE:O	2:G:608:ASP:N	2.54	0.41
1:B:17:ILE:O	1:B:18:LYS:C	2.64	0.40
1:B:88:VAL:HA	1:B:89:PRO:HD2	1.75	0.40
1:C:78:VAL:O	1:C:82:LEU:CB	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:SER:O	1:C:399:GLY:N	2.54	0.40
1:D:150:VAL:O	1:D:156:ALA:HA	2.21	0.40
2:E:470:LEU:HD13	2:E:518:LEU:HD13	2.03	0.40
2:E:542:SER:C	2:E:543:ILE:HG12	2.46	0.40
2:E:544:ILE:HG21	2:E:563:ILE:HD11	2.04	0.40
2:G:542:SER:C	2:G:543:ILE:HG12	2.46	0.40
2:G:563:ILE:H	2:G:563:ILE:HG13	1.59	0.40
2:H:540:HIS:HB2	2:H:587:GLN:HG3	2.03	0.40
2:H:570:VAL:HG12	2:H:591:CYS:HA	2.03	0.40
1:A:110:VAL:HG23	1:A:112:ILE:HD11	2.03	0.40
1:A:294:ILE:HG12	1:A:301:TYR:CD1	2.56	0.40
1:C:401:GLN:OE1	2:G:548:TYR:HB2	2.21	0.40
2:H:471:VAL:HG13	2:H:477:HIS:H	1.85	0.40
2:H:548:TYR:OH	2:H:624:ILE:HG21	2.21	0.40
1:A:377:TRP:CH2	1:A:385:PHE:HE2	2.40	0.40
1:B:45:ILE:O	1:B:46:SER:C	2.64	0.40
1:B:152:ASP:HB3	1:B:155:GLY:O	2.22	0.40
1:D:396:SER:O	1:D:399:GLY:N	2.53	0.40
2:E:538:ILE:O	2:E:539:GLU:C	2.65	0.40
2:F:442:LEU:HD12	2:F:458:LYS:C	2.47	0.40
2:H:543:ILE:O	2:H:544:ILE:HG13	2.22	0.40
1:A:22:LYS:O	1:A:24:LEU:N	2.54	0.40
1:A:45:ILE:O	1:A:46:SER:C	2.63	0.40
1:A:76:THR:O	1:A:77:SER:C	2.63	0.40
1:B:89:PRO:HA	1:B:90:PRO:HD2	1.87	0.40
1:D:166:ARG:O	1:D:167:GLU:HG3	2.21	0.40
1:D:279:LYS:O	1:D:283:GLU:HB2	2.22	0.40
2:E:577:LYS:HB3	2:E:577:LYS:HE2	1.87	0.40
2:F:520:ASP:OD1	2:F:521:PRO:HD2	2.21	0.40
1:A:279:LYS:H	1:A:279:LYS:CD	2.18	0.40
1:C:306:GLU:O	1:C:307:ASP:C	2.64	0.40
1:D:307:ASP:O	1:D:311:ALA:N	2.52	0.40
2:E:470:LEU:N	2:E:479:VAL:O	2.54	0.40
2:F:473:MET:CE	2:F:525:CYS:HB2	2.51	0.40
2:G:533:ALA:HB1	2:G:629:VAL:HA	2.03	0.40
2:H:444:ILE:HD12	2:H:516:PHE:HB2	2.04	0.40
2:H:563:ILE:H	2:H:563:ILE:HG13	1.59	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	374/451 (83%)	289 (77%)	55 (15%)	30 (8%)	1	10
1	B	374/451 (83%)	290 (78%)	51 (14%)	33 (9%)	0	9
1	C	298/451 (66%)	230 (77%)	51 (17%)	17 (6%)	1	15
1	D	298/451 (66%)	229 (77%)	52 (17%)	17 (6%)	1	15
2	E	193/204 (95%)	143 (74%)	34 (18%)	16 (8%)	0	9
2	F	193/204 (95%)	146 (76%)	30 (16%)	17 (9%)	0	9
2	G	193/204 (95%)	148 (77%)	31 (16%)	14 (7%)	1	11
2	H	193/204 (95%)	148 (77%)	31 (16%)	14 (7%)	1	11
All	All	2116/2620 (81%)	1623 (77%)	335 (16%)	158 (8%)	1	11

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	108	LYS
1	A	115	GLU
1	A	116	PRO
1	A	118	LYS
1	A	120	ILE
1	A	122	THR
1	A	142	ASP
1	A	177	PRO
1	A	222	ALA
1	A	276	SER
1	A	347	THR
1	A	381	ASN
1	B	65	ARG
1	B	108	LYS
1	B	115	GLU
1	B	116	PRO

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Mol	Chain	Res	Type
1	B	118	LYS
1	B	120	ILE
1	B	122	THR
1	B	142	ASP
1	B	177	PRO
1	B	222	ALA
1	B	276	SER
1	B	347	THR
1	B	381	ASN
1	B	416	ARG
1	C	116	PRO
1	C	409	ILE
1	D	116	PRO
1	D	409	ILE
2	E	489	VAL
2	E	510	GLU
2	E	538	ILE
2	E	540	HIS
2	E	567	ILE
2	F	489	VAL
2	F	510	GLU
2	F	538	ILE
2	F	540	HIS
2	F	567	ILE
2	G	489	VAL
2	G	540	HIS
2	H	489	VAL
2	H	540	HIS
1	A	90	PRO
1	A	117	PHE
1	A	119	PRO
1	A	163	GLY
1	B	117	PHE
1	B	119	PRO
1	B	163	GLY
1	C	222	ALA
1	C	273	GLU
1	C	306	GLU
1	C	318	GLU
1	D	222	ALA
1	D	273	GLU
1	D	306	GLU

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Mol	Chain	Res	Type
1	D	318	GLU
2	E	523	ASN
2	E	564	THR
2	F	523	ASN
2	F	539	GLU
2	F	564	THR
2	G	487	ASP
2	G	518	LEU
2	G	523	ASN
2	G	556	THR
2	G	559	GLU
2	H	487	ASP
2	H	518	LEU
2	H	523	ASN
2	H	556	THR
2	H	559	GLU
1	A	184	GLY
1	A	258	TYR
1	A	272	THR
1	A	388	THR
1	B	90	PRO
1	B	184	GLY
1	B	258	TYR
1	B	272	THR
1	B	388	THR
1	C	154	SER
1	C	229	SER
1	C	272	THR
1	C	381	ASN
1	D	154	SER
1	D	229	SER
1	D	272	THR
1	D	327	ASP
1	D	381	ASN
1	D	416	ARG
2	E	469	GLN
2	E	487	ASP
2	E	555	HIS
2	E	557	CYS
2	F	469	GLN
2	F	487	ASP
2	F	555	HIS

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Mol	Chain	Res	Type
2	G	475	ASN
1	A	69	LEU
1	A	183	GLY
1	A	229	SER
1	A	240	ASP
1	B	23	SER
1	B	69	LEU
1	B	183	GLY
1	B	240	ASP
1	C	327	ASP
1	C	388	THR
1	D	388	THR
2	E	518	LEU
2	E	598	ALA
2	F	557	CYS
2	G	521	PRO
2	G	538	ILE
2	G	574	SER
2	H	475	ASN
2	H	521	PRO
2	H	538	ILE
2	H	574	SER
1	A	23	SER
1	A	190	PHE
1	A	224	LEU
1	B	190	PHE
1	B	224	LEU
1	B	229	SER
1	C	221	VAL
1	D	221	VAL
1	D	398	GLU
2	E	521	PRO
2	F	518	LEU
2	F	521	PRO
2	F	598	ALA
2	G	470	LEU
2	G	537	ILE
2	G	567	ILE
2	H	470	LEU
2	H	567	ILE
1	A	221	VAL
1	B	68	ARG

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Mol	Chain	Res	Type
1	B	221	VAL
1	C	299	GLY
1	C	398	GLU
1	D	299	GLY
2	H	537	ILE
2	E	554	ILE
2	F	554	ILE
1	C	347	THR
1	D	347	THR
2	E	558	ILE
2	F	558	ILE
1	B	31	GLY
1	B	348	PRO
1	A	348	PRO
1	C	73	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	325/387 (84%)	264 (81%)	61 (19%)	1	10
1	B	325/387 (84%)	263 (81%)	62 (19%)	1	9
1	C	275/387 (71%)	242 (88%)	33 (12%)	5	21
1	D	275/387 (71%)	244 (89%)	31 (11%)	5	23
2	E	173/180 (96%)	134 (78%)	39 (22%)	1	5
2	F	173/180 (96%)	132 (76%)	41 (24%)	1	5
2	G	173/180 (96%)	135 (78%)	38 (22%)	1	5
2	H	173/180 (96%)	135 (78%)	38 (22%)	1	5
All	All	1892/2268 (83%)	1549 (82%)	343 (18%)	2	12

All (343) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	22	LYS
1	A	25	GLU
1	A	28	ARG
1	A	35	ILE
1	A	38	ILE
1	A	60	SER
1	A	62	ILE
1	A	63	LYS
1	A	65	ARG
1	A	70	SER
1	A	78	VAL
1	A	79	GLN
1	A	84	LEU
1	A	86	ASN
1	A	93	LEU
1	A	95	VAL
1	A	101	VAL
1	A	110	VAL
1	A	118	LYS
1	A	120	ILE
1	A	122	THR
1	A	124	LEU
1	A	126	LEU
1	A	127	CYS
1	A	141	SER
1	A	145	LYS
1	A	165	THR
1	A	166	ARG
1	A	168	VAL
1	A	178	LYS
1	A	185	GLN
1	A	192	ARG
1	A	200	ASN
1	A	211	GLN
1	A	214	ILE
1	A	218	LYS
1	A	239	SER
1	A	240	ASP
1	A	241	MET
1	A	244	GLN
1	A	251	LEU
1	A	274	VAL

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Mol	Chain	Res	Type
1	A	276	SER
1	A	279	LYS
1	A	291	PHE
1	A	294	ILE
1	A	300	LYS
1	A	303	PHE
1	A	306	GLU
1	A	317	VAL
1	A	326	LEU
1	A	327	ASP
1	A	328	ILE
1	A	346	LEU
1	A	374	LEU
1	A	385	PHE
1	A	389	LEU
1	A	395	LYS
1	A	403	VAL
1	A	404	LYS
1	B	10	ARG
1	B	22	LYS
1	B	25	GLU
1	B	28	ARG
1	B	35	ILE
1	B	38	ILE
1	B	60	SER
1	B	62	ILE
1	B	63	LYS
1	B	65	ARG
1	B	70	SER
1	B	78	VAL
1	B	79	GLN
1	B	84	LEU
1	B	86	ASN
1	B	93	LEU
1	B	95	VAL
1	B	101	VAL
1	B	110	VAL
1	B	118	LYS
1	B	120	ILE
1	B	122	THR
1	B	124	LEU
1	B	126	LEU

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Mol	Chain	Res	Type
1	B	127	CYS
1	B	139	LEU
1	B	141	SER
1	B	145	LYS
1	B	165	THR
1	B	166	ARG
1	B	168	VAL
1	B	178	LYS
1	B	185	GLN
1	B	192	ARG
1	B	200	ASN
1	B	211	GLN
1	B	214	ILE
1	B	218	LYS
1	B	239	SER
1	B	241	MET
1	B	244	GLN
1	B	251	LEU
1	B	274	VAL
1	B	276	SER
1	B	279	LYS
1	B	291	PHE
1	B	294	ILE
1	B	300	LYS
1	B	303	PHE
1	B	306	GLU
1	B	317	VAL
1	B	326	LEU
1	B	327	ASP
1	B	328	ILE
1	B	346	LEU
1	B	374	LEU
1	B	385	PHE
1	B	389	LEU
1	B	395	LYS
1	B	403	VAL
1	B	404	LYS
1	B	420	GLN
1	C	23	SER
1	C	39	ILE
1	C	51	MET
1	C	67	ASN

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Mol	Chain	Res	Type
1	C	117	PHE
1	C	118	LYS
1	C	144	SER
1	C	150	VAL
1	C	161	LEU
1	C	166	ARG
1	C	198	ARG
1	C	199	HIS
1	C	208	THR
1	C	211	GLN
1	C	214	ILE
1	C	218	LYS
1	C	221	VAL
1	C	233	LYS
1	C	237	SER
1	C	251	LEU
1	C	272	THR
1	C	275	LEU
1	C	300	LYS
1	C	305	VAL
1	C	329	MET
1	C	374	LEU
1	C	391	ILE
1	C	397	GLN
1	C	398	GLU
1	C	413	LEU
1	C	414	ARG
1	C	415	TYR
1	C	416	ARG
1	D	23	SER
1	D	39	ILE
1	D	51	MET
1	D	67	ASN
1	D	117	PHE
1	D	118	LYS
1	D	144	SER
1	D	150	VAL
1	D	161	LEU
1	D	166	ARG
1	D	173	THR
1	D	198	ARG
1	D	199	HIS

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Mol	Chain	Res	Type
1	D	208	THR
1	D	211	GLN
1	D	214	ILE
1	D	218	LYS
1	D	221	VAL
1	D	233	LYS
1	D	251	LEU
1	D	272	THR
1	D	275	LEU
1	D	300	LYS
1	D	305	VAL
1	D	329	MET
1	D	374	LEU
1	D	391	ILE
1	D	397	GLN
1	D	398	GLU
1	D	413	LEU
1	D	416	ARG
2	E	440	ILE
2	E	441	ARG
2	E	448	TYR
2	E	453	THR
2	E	459	LEU
2	E	464	ILE
2	E	470	LEU
2	E	471	VAL
2	E	476	LYS
2	E	490	GLU
2	E	500	LEU
2	E	502	ILE
2	E	508	GLU
2	E	511	GLU
2	E	517	ILE
2	E	520	ASP
2	E	524	LEU
2	E	540	HIS
2	E	543	ILE
2	E	555	HIS
2	E	558	ILE
2	E	566	LEU
2	E	570	VAL
2	E	574	SER

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Mol	Chain	Res	Type
2	E	577	LYS
2	E	586	LYS
2	E	592	ILE
2	E	597	THR
2	E	603	LEU
2	E	607	LYS
2	E	608	ASP
2	E	612	MET
2	E	616	THR
2	E	617	LEU
2	E	622	LYS
2	E	624	ILE
2	E	626	ILE
2	E	629	VAL
2	E	633	VAL
2	F	440	ILE
2	F	441	ARG
2	F	448	TYR
2	F	453	THR
2	F	459	LEU
2	F	464	ILE
2	F	470	LEU
2	F	471	VAL
2	F	475	ASN
2	F	476	LYS
2	F	490	GLU
2	F	500	LEU
2	F	502	ILE
2	F	508	GLU
2	F	511	GLU
2	F	517	ILE
2	F	520	ASP
2	F	524	LEU
2	F	538	ILE
2	F	540	HIS
2	F	543	ILE
2	F	555	HIS
2	F	558	ILE
2	F	566	LEU
2	F	570	VAL
2	F	574	SER
2	F	577	LYS

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Mol	Chain	Res	Type
2	F	586	LYS
2	F	592	ILE
2	F	597	THR
2	F	603	LEU
2	F	607	LYS
2	F	608	ASP
2	F	612	MET
2	F	616	THR
2	F	617	LEU
2	F	622	LYS
2	F	624	ILE
2	F	626	ILE
2	F	629	VAL
2	F	633	VAL
2	G	440	ILE
2	G	453	THR
2	G	459	LEU
2	G	464	ILE
2	G	470	LEU
2	G	476	LYS
2	G	487	ASP
2	G	490	GLU
2	G	492	ASP
2	G	494	VAL
2	G	500	LEU
2	G	502	ILE
2	G	503	ARG
2	G	510	GLU
2	G	512	ILE
2	G	520	ASP
2	G	536	VAL
2	G	538	ILE
2	G	543	ILE
2	G	552	LEU
2	G	558	ILE
2	G	563	ILE
2	G	566	LEU
2	G	570	VAL
2	G	574	SER
2	G	579	LYS
2	G	590	VAL
2	G	592	ILE

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Mol	Chain	Res	Type
2	G	612	MET
2	G	614	ARG
2	G	616	THR
2	G	617	LEU
2	G	620	GLU
2	G	622	LYS
2	G	624	ILE
2	G	626	ILE
2	G	632	LEU
2	G	633	VAL
2	H	440	ILE
2	H	453	THR
2	H	459	LEU
2	H	464	ILE
2	H	470	LEU
2	H	476	LYS
2	H	487	ASP
2	H	490	GLU
2	H	491	THR
2	H	492	ASP
2	H	494	VAL
2	H	500	LEU
2	H	502	ILE
2	H	503	ARG
2	H	510	GLU
2	H	512	ILE
2	H	520	ASP
2	H	536	VAL
2	H	538	ILE
2	H	543	ILE
2	H	552	LEU
2	H	558	ILE
2	H	563	ILE
2	H	566	LEU
2	H	570	VAL
2	H	574	SER
2	H	579	LYS
2	H	590	VAL
2	H	592	ILE
2	H	612	MET
2	H	614	ARG
2	H	616	THR

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Mol	Chain	Res	Type
2	H	617	LEU
2	H	620	GLU
2	H	622	LYS
2	H	626	ILE
2	H	632	LEU
2	H	633	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	164	ASN
1	A	185	GLN
1	A	200	ASN
1	A	244	GLN
1	A	266	GLN
1	A	397	GLN
1	B	11	ASN
1	B	111	ASN
1	B	164	ASN
1	B	185	GLN
1	B	200	ASN
1	B	244	GLN
1	B	266	GLN
1	B	282	GLN
1	B	397	GLN
1	B	420	GLN
1	C	121	ASN
1	C	162	GLN
1	C	244	GLN
1	C	266	GLN
1	C	350	GLN
1	C	381	ASN
1	D	121	ASN
1	D	162	GLN
1	D	244	GLN
1	D	266	GLN
1	D	350	GLN
1	D	381	ASN
2	E	477	HIS
2	E	549	ASN
2	E	587	GLN

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Mol	Chain	Res	Type
2	F	477	HIS
2	F	549	ASN
2	F	587	GLN
2	G	469	GLN
2	G	477	HIS
2	H	469	GLN
2	H	534	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 ⓘ

2 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
3	ATP	A	1526	-	32,33,33	1.50	7 (21%)	48,52,52	1.87	8 (16%)
3	ATP	B	1526	-	32,33,33	1.53	7 (21%)	48,52,52	1.78	6 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1526	-	-	5/22/38/38	0/3/3/3
3	ATP	B	1526	-	-	3/22/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1526	ATP	C5-C4	5.12	1.48	1.39
3	B	1526	ATP	C5-C4	5.04	1.48	1.39
3	B	1526	ATP	PB-O3A	2.85	1.62	1.59
3	A	1526	ATP	C5-C6	2.71	1.48	1.41
3	B	1526	ATP	C5-C6	2.63	1.48	1.41
3	A	1526	ATP	C5-N7	-2.49	1.34	1.39
3	B	1526	ATP	C5-N7	-2.49	1.34	1.39
3	B	1526	ATP	PB-O3B	2.34	1.62	1.59
3	A	1526	ATP	C8-N7	2.27	1.36	1.31
3	A	1526	ATP	PA-O3A	2.22	1.61	1.59
3	A	1526	ATP	PB-O3B	2.22	1.61	1.59
3	B	1526	ATP	PA-O3A	2.13	1.61	1.59
3	B	1526	ATP	C8-N7	2.12	1.35	1.31
3	A	1526	ATP	PB-O3A	2.05	1.61	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1526	ATP	C5-C4-N3	-6.94	117.16	126.72
3	B	1526	ATP	C5-C4-N3	-6.41	117.89	126.72
3	B	1526	ATP	N3-C4-N9	5.29	136.16	127.17
3	A	1526	ATP	N3-C4-N9	5.23	136.06	127.17
3	A	1526	ATP	C2-N3-C4	4.00	121.59	111.83
3	B	1526	ATP	C2-N3-C4	3.77	121.05	111.83
3	A	1526	ATP	C4-C5-N7	-3.32	106.79	110.58
3	B	1526	ATP	N3-C2-N1	-3.04	123.99	128.58
3	A	1526	ATP	N3-C2-N1	-3.00	124.04	128.58
3	B	1526	ATP	C4-C5-N7	-2.96	107.20	110.58
3	A	1526	ATP	C3'-C2'-C1'	2.46	106.12	101.46
3	A	1526	ATP	O4'-C1'-N9	2.46	112.81	108.09
3	A	1526	ATP	C5-N7-C8	2.17	106.85	103.45
3	B	1526	ATP	C5-N7-C8	2.07	106.70	103.45

There are no chirality outliers.

All (8) torsion outliers are listed below:

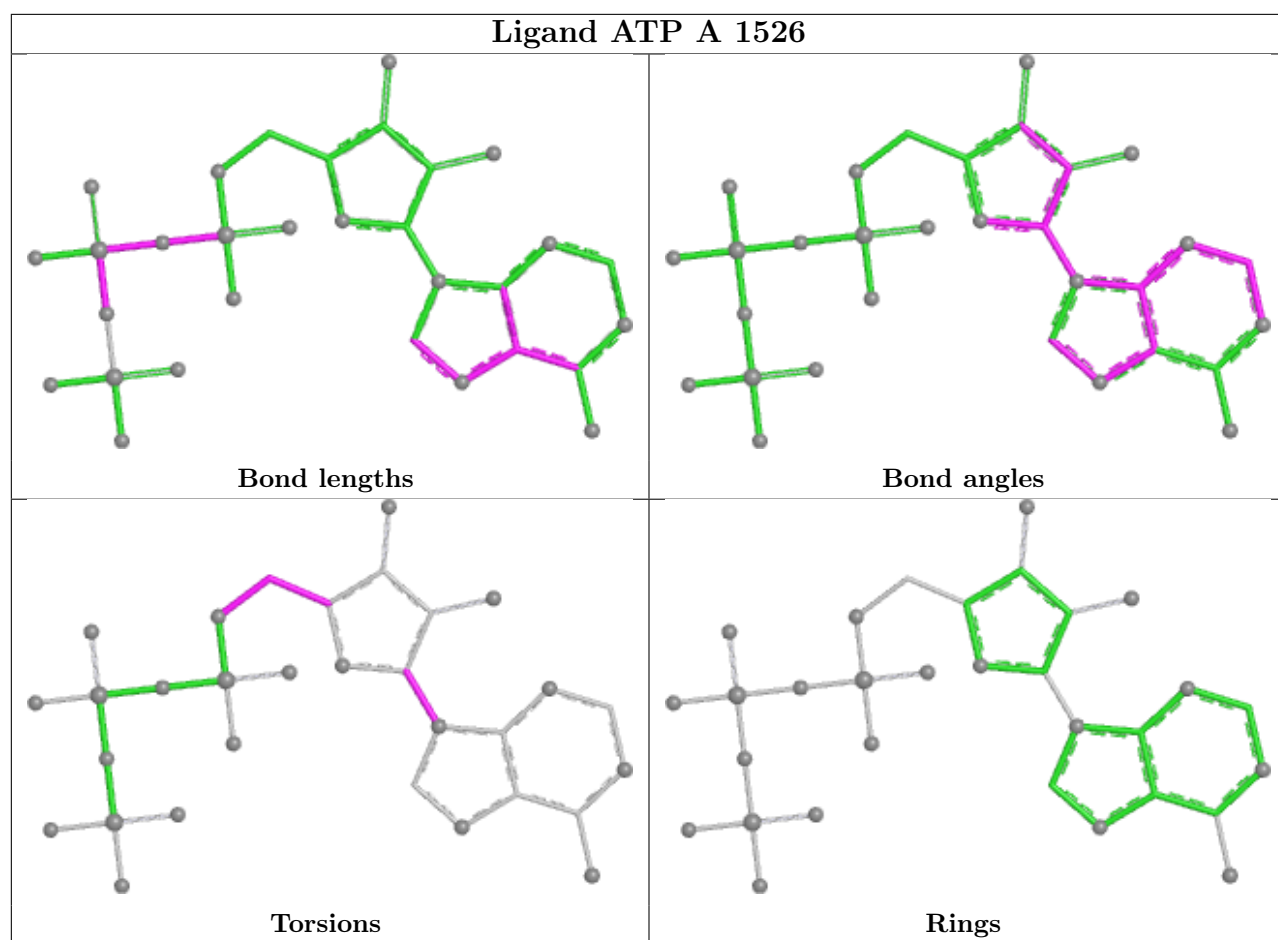
Mol	Chain	Res	Type	Atoms
3	A	1526	ATP	O4'-C1'-N9-C8
3	A	1526	ATP	O4'-C1'-N9-C4
3	A	1526	ATP	C3'-C4'-C5'-O5'
3	A	1526	ATP	O4'-C4'-C5'-O5'
3	A	1526	ATP	C4'-C5'-O5'-PA
3	B	1526	ATP	O4'-C1'-N9-C8
3	B	1526	ATP	PA-O3A-PB-O2B
3	B	1526	ATP	PB-O3A-PA-O2A

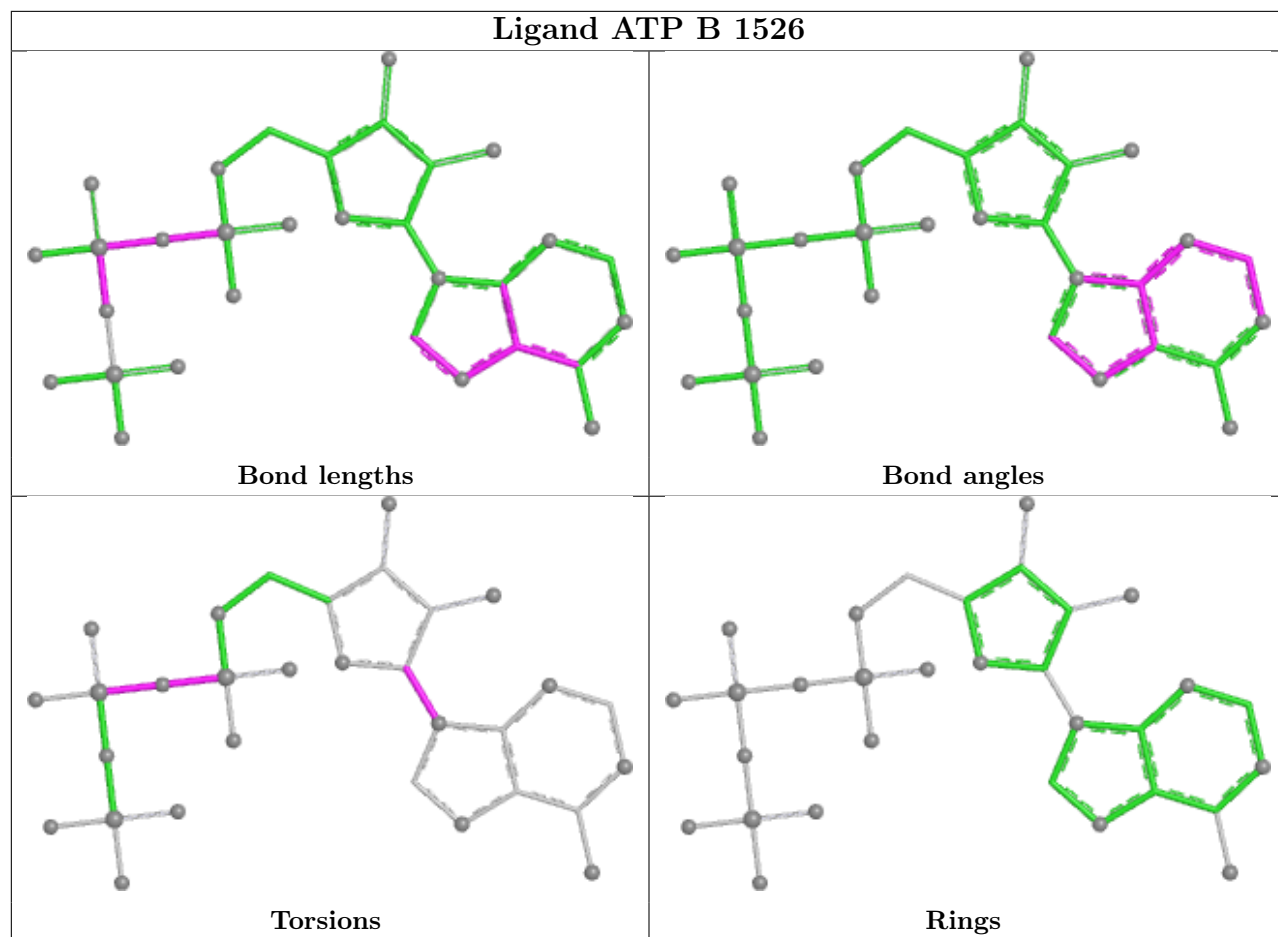
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1526	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	380/451 (84%)	-0.65	2 (0%) 87 71	71, 89, 96, 100	0
1	B	380/451 (84%)	-0.66	3 (0%) 82 62	71, 89, 96, 100	0
1	C	318/451 (70%)	-0.51	3 (0%) 81 60	73, 90, 93, 100	0
1	D	318/451 (70%)	-0.52	4 (1%) 75 53	73, 90, 93, 100	0
2	E	195/204 (95%)	-0.62	0 100 100	56, 87, 93, 97	0
2	F	195/204 (95%)	-0.65	1 (0%) 87 71	56, 87, 93, 97	0
2	G	195/204 (95%)	-0.53	2 (1%) 79 58	55, 87, 92, 96	0
2	H	195/204 (95%)	-0.49	1 (0%) 87 71	55, 87, 92, 96	0
All	All	2176/2620 (83%)	-0.58	16 (0%) 84 65	55, 89, 95, 100	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	257	SER	5.4
1	C	125	TYR	5.3
1	C	327	ASP	3.6
1	D	327	ASP	3.6
1	A	180	HIS	3.5
1	B	104	GLU	3.2
2	G	493	THR	3.1
1	A	274	VAL	3.0
1	B	257	SER	3.0
1	B	163	GLY	3.0
2	H	462	GLY	2.8
1	D	141	SER	2.6
2	G	507	ILE	2.5
1	D	258	TYR	2.3
2	F	539	GLU	2.3
1	C	258	TYR	2.2

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](#)

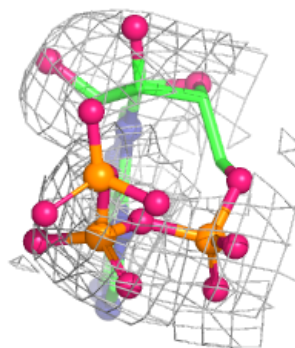
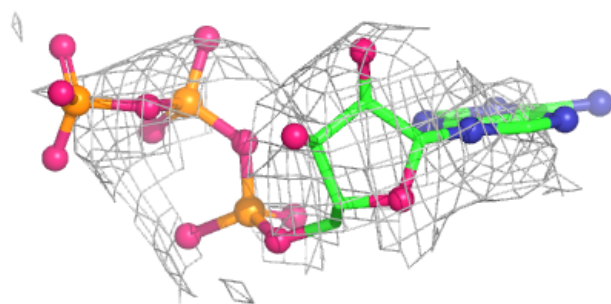
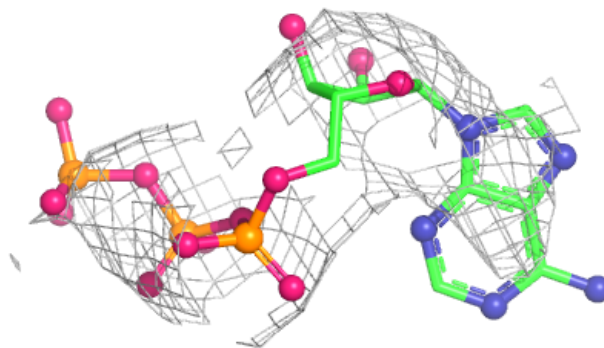
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	B	1526	31/31	0.97	0.08	169,171,179,179	0
3	ATP	A	1526	31/31	0.99	0.06	171,173,180,180	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

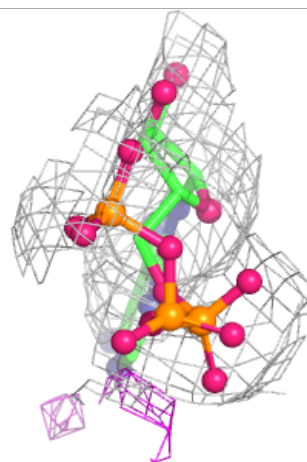
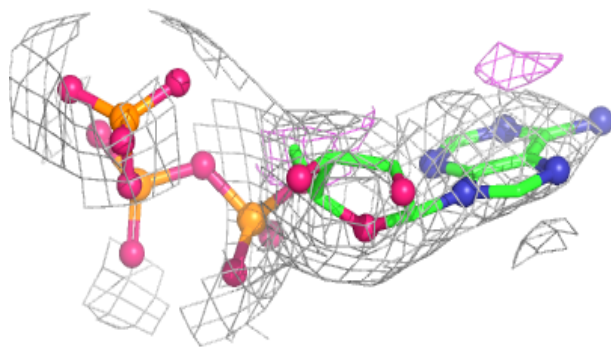
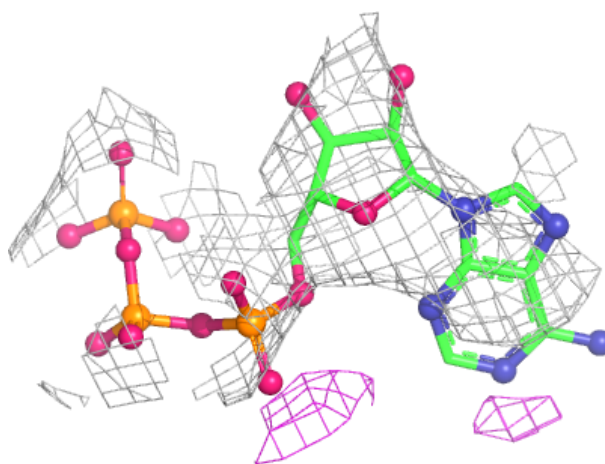
Electron density around ATP B 1526:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP A 1526:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.