



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:27 PM UTC

PDB ID : 2A45 / pdb_00002a45
Title : Crystal structure of the complex between thrombin and the central "E" region of fibrin
Authors : Pechik, I.; Madrazo, J.; Gilliland, G.L.; Medved, L.
Deposited on : 2005-06-27
Resolution : 3.65 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

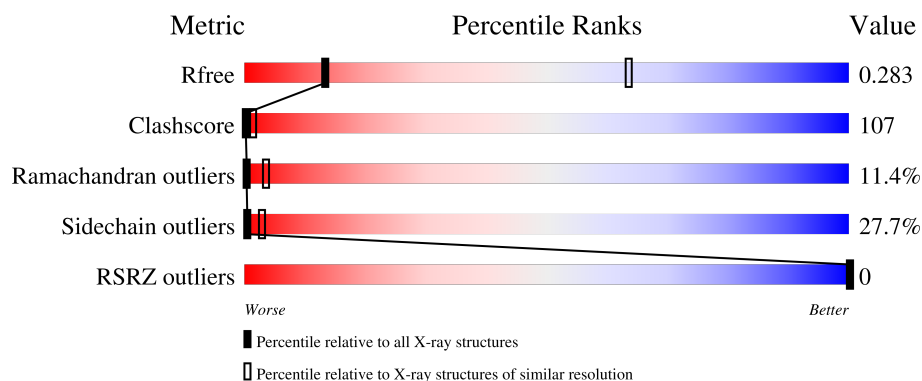
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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	36	
1	D	36	
2	B	259	
2	E	259	
3	G	57	

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Mol	Chain	Length	Quality of chain
3	J	57	
4	H	91	
4	K	91	
5	I	45	
5	L	45	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	0G6	B	1	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6904 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 Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	32	Total	C	N	O	S	0	0	0
			259	159	44	55	1			
1	D	32	Total	C	N	O	S	0	0	0
			259	159	44	55	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2069	1320	364	371	14			
2	E	258	Total	C	N	O	S	0	0	0
			2069	1320	364	371	14			

- Molecule 3 is a protein called Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	48	Total	C	N	O	S	17	0	0
			384	235	67	77	5			
3	J	48	Total	C	N	O	S	17	0	0
			384	235	67	77	5			

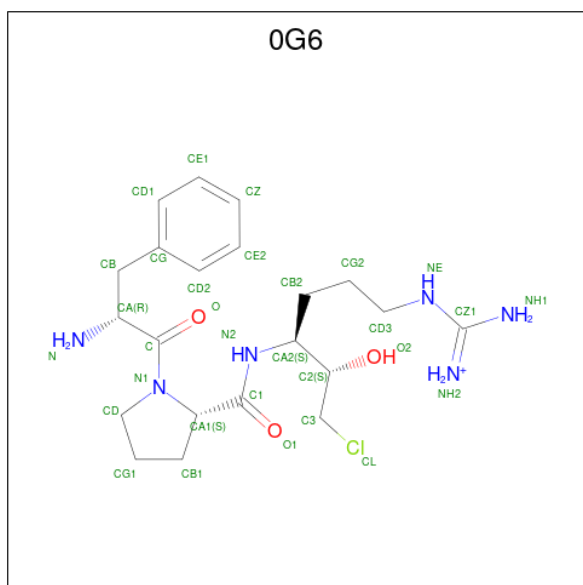
- Molecule 4 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	52	Total	C	N	O	S	0	0	0
			382	230	72	77	3			
4	K	52	Total	C	N	O	S	0	0	0
			382	230	72	77	3			

- Molecule 5 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	40	Total	C	N	O	S	0	0	0
			308	189	47	68	4			
5	L	44	Total	C	N	O	S	0	0	0
			338	207	54	73	4			

- Molecule 6 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (CCD ID: 0G6) (formula: $C_{21}H_{34}ClN_6O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			30	21	6	3		
6	E	1	Total	C	N	O	0	0
			30	21	6	3		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

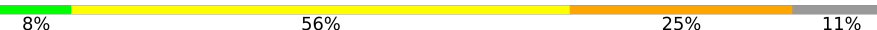


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	0
			5	4	1		
7	E	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Thrombin light chain

Chain A: 



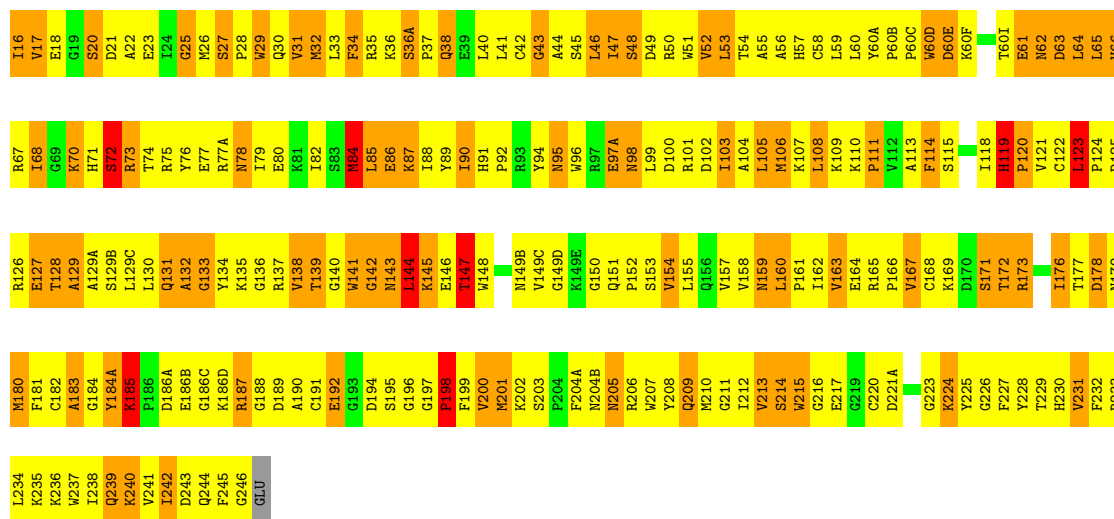
- Molecule 1: Thrombin light chain

Chain D: 

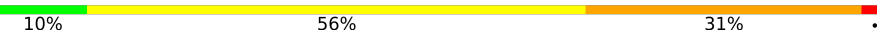


- Molecule 2: Thrombin heavy chain

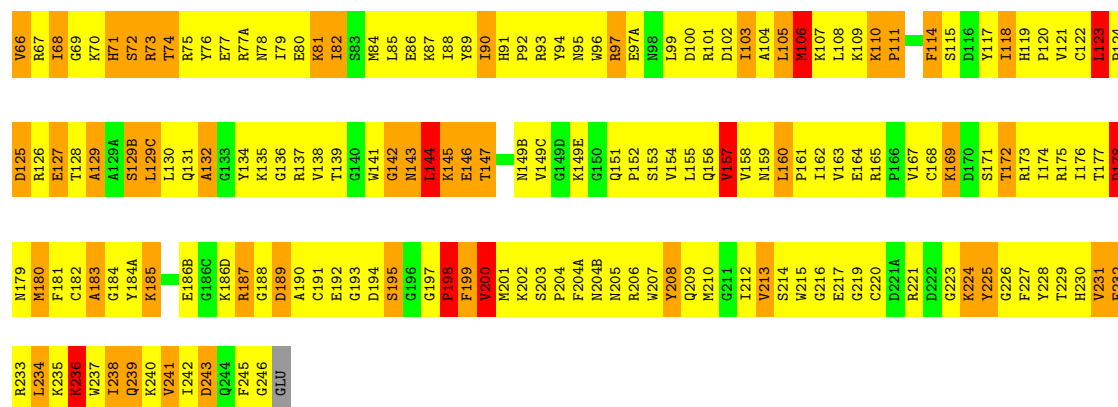
Chain B: 



- Molecule 2: Thrombin heavy chain

Chain E: 





- Molecule 3: Fibrinogen alpha chain

Chain G: 11% 44% 26% • 16%



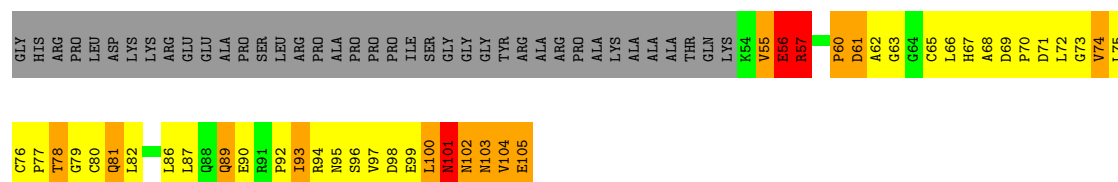
- Molecule 3: Fibrinogen alpha chain

Chain J: 9% 51% 19% 5% 16%



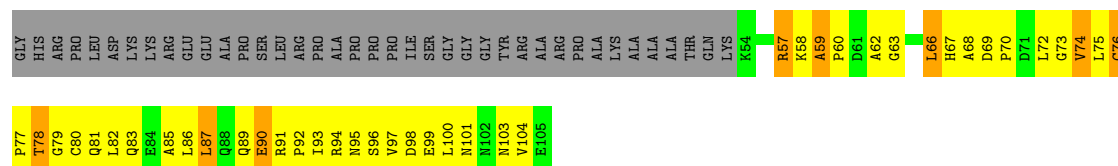
- Molecule 4: Fibrinogen beta chain

Chain H: 10% 30% 14% • 43%



- Molecule 4: Fibrinogen beta chain

Chain K: 12% 36% 9% 43%



- Molecule 5: Fibrinogen gamma chain

Chain I: 9% 42% 31% 7% 11%



● Molecule 5: Fibrinogen gamma chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	76.26Å 76.26Å 192.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.70 – 3.65 19.70 – 3.65	Depositor EDS
% Data completeness (in resolution range)	93.4 (19.70-3.65) 97.5 (19.70-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.24Å)	Xtriage
Refinement program	CNS 1.1, SHELXL-97	Depositor
R, R_{free}	0.221 , 0.290 0.214 , 0.283	Depositor DCC
R_{free} test set	2442 reflections (6.55%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.088 for -h,-k,l 0.347 for h,-h-k,-l 0.089 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6904	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: 0G6, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	0/261	1.13	1/345 (0.3%)
1	D	0.79	1/261 (0.4%)	1.13	0/345
2	B	0.76	0/2124	1.25	25/2876 (0.9%)
2	E	0.79	0/2124	1.21	22/2876 (0.8%)
3	G	0.79	0/392	1.43	10/527 (1.9%)
3	J	0.76	0/392	1.34	6/527 (1.1%)
4	H	0.93	2/386 (0.5%)	1.26	1/524 (0.2%)
4	K	0.83	0/386	1.25	6/524 (1.1%)
5	I	0.85	0/312	1.14	2/423 (0.5%)
5	L	0.79	0/342	1.15	2/464 (0.4%)
All	All	0.79	3/6980 (0.0%)	1.24	75/9431 (0.8%)

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
5	L	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	56	GLU	CA-C	7.30	1.55	1.52
1	D	14(K)	ILE	CA-CB	6.36	1.63	1.54
4	H	55	VAL	CA-CB	5.21	1.60	1.54

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	55	VAL	N-CA-C	9.65	122.16	112.90
3	J	28	CYS	N-CA-C	9.27	130.55	110.80
3	G	28	CYS	N-CA-C	8.51	128.93	110.80
2	E	43	GLY	N-CA-C	-8.14	101.59	112.82
2	B	43	GLY	N-CA-C	-7.98	98.89	111.18
2	B	84	MET	N-CA-C	-7.20	101.56	110.41
2	B	173	ARG	N-CA-C	-7.18	103.68	113.30
5	L	23	CYS	N-CA-C	-7.12	103.21	110.97
2	E	52	VAL	N-CA-C	7.06	117.67	108.35
1	A	1(B)	ALA	N-CA-C	-6.98	103.86	113.56
3	J	45	CYS	CA-C-N	6.98	128.56	119.84
3	J	45	CYS	C-N-CA	6.98	128.56	119.84
2	B	97(A)	GLU	N-CA-C	6.97	118.67	111.14
2	B	119	HIS	CA-C-N	6.63	126.81	120.31
2	B	119	HIS	C-N-CA	6.63	126.81	120.31
3	G	45	CYS	CA-C-N	6.61	128.10	119.84
3	G	45	CYS	C-N-CA	6.61	128.10	119.84
3	G	33	TRP	CA-C-N	6.60	128.09	119.84
3	G	33	TRP	C-N-CA	6.60	128.09	119.84
2	E	160	LEU	CA-C-N	6.56	126.94	119.92
2	E	160	LEU	C-N-CA	6.56	126.94	119.92
4	K	74	VAL	N-CA-C	6.47	117.78	109.30
2	B	60(D)	TRP	N-CA-C	-6.45	106.14	112.97
5	L	33	GLN	N-CA-C	6.33	118.70	111.11
2	B	185	LYS	CA-C-N	6.28	126.75	119.47
2	B	185	LYS	C-N-CA	6.28	126.75	119.47
2	B	223	GLY	N-CA-C	-6.24	106.51	114.37
2	E	200	VAL	CB-CA-C	-6.10	104.88	111.59
3	J	33	TRP	N-CA-C	6.10	118.32	110.39
3	J	28	CYS	CA-CB-SG	-6.04	100.52	114.40
3	G	54	LEU	N-CA-C	-6.03	104.05	111.40
2	E	157	VAL	N-CA-C	5.94	118.18	108.97
2	B	148	TRP	N-CA-C	5.89	121.50	113.37
3	G	31	SER	CB-CA-C	-5.87	109.82	116.63
3	G	28	CYS	CA-CB-SG	-5.86	100.93	114.40
2	B	141	TRP	N-CA-C	-5.83	106.21	113.15
2	E	71	HIS	N-CA-C	-5.80	106.12	113.43
4	K	97	VAL	N-CA-C	5.75	115.83	110.42
2	B	160	LEU	CA-C-N	5.71	125.62	119.85
2	B	160	LEU	C-N-CA	5.71	125.62	119.85
2	E	147	THR	N-CA-C	5.69	122.91	110.80
2	E	28	PRO	N-CA-C	-5.68	108.17	114.92
2	B	123	LEU	CA-C-N	5.67	125.69	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	123	LEU	C-N-CA	5.67	125.69	119.90
2	B	163	VAL	N-CA-C	5.67	116.75	108.53
2	B	72	SER	N-CA-C	-5.58	101.39	110.20
2	E	208	TYR	N-CA-C	5.53	117.45	108.26
5	I	28	PHE	N-CA-C	-5.45	105.44	111.71
2	E	118	ILE	N-CA-C	5.45	115.70	107.80
2	B	209	GLN	N-CA-C	-5.44	100.43	109.46
2	B	29	TRP	N-CA-C	-5.39	106.58	114.39
2	E	106	MET	N-CA-C	5.37	117.42	108.99
2	E	82	ILE	CB-CA-C	-5.33	104.38	110.73
3	G	43	TYR	N-CA-C	-5.30	105.09	112.30
2	E	245	PHE	N-CA-C	5.30	119.08	111.02
2	E	199	PHE	N-CA-C	-5.27	98.42	108.17
4	K	76	CYS	CA-C-N	5.27	125.57	119.93
4	K	76	CYS	C-N-CA	5.27	125.57	119.93
2	E	178	ASP	N-CA-C	-5.26	106.71	113.23
5	I	31	THR	N-CA-C	-5.26	104.46	111.24
2	E	172	THR	N-CA-C	5.23	117.34	109.23
4	K	59	ALA	CA-C-N	5.23	127.31	120.25
4	K	59	ALA	C-N-CA	5.23	127.31	120.25
3	G	71	ASN	N-CA-C	5.22	116.78	111.14
2	B	25	GLY	N-CA-C	5.19	122.01	115.42
2	B	138	VAL	N-CA-C	-5.13	102.27	108.53
2	E	144	LEU	N-CA-C	5.11	121.68	110.80
2	B	66	VAL	N-CA-C	5.10	115.31	108.17
2	E	123	LEU	CA-C-N	5.09	125.09	119.90
2	E	123	LEU	C-N-CA	5.09	125.09	119.90
2	E	24	ILE	N-CA-C	5.09	115.42	107.99
3	J	29	LYS	N-CA-C	5.05	121.56	110.80
2	B	215	TRP	N-CA-C	5.05	114.90	108.24
2	B	147	THR	N-CA-C	5.03	121.52	110.80
2	E	66	VAL	N-CA-C	5.00	115.32	108.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	32	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	259	0	254	61	0
1	D	259	0	254	50	0
2	B	2069	0	2024	522	0
2	E	2069	0	2024	468	0
3	G	384	0	348	77	0
3	J	384	0	348	91	0
4	H	382	0	362	82	0
4	K	382	0	362	72	0
5	I	308	0	273	72	0
5	L	338	0	307	67	0
6	B	30	0	30	33	0
6	E	30	0	30	19	0
7	B	5	0	0	0	0
7	E	5	0	0	0	0
All	All	6904	0	6616	1446	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 107.

All (1446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD23	1:A:13:GLU:H	1.09	1.17
4:K:98:ASP:HA	4:K:101:ASN:HD21	1.09	1.16
2:E:99:LEU:HD11	6:E:1:OG6:HB21	1.20	1.13
2:E:60(A):TYR:H	2:E:60(F):LYS:HB3	1.07	1.12
2:E:138:VAL:HG22	2:E:199:PHE:HA	1.26	1.10
2:E:31:VAL:HB	2:E:44:ALA:HB3	1.26	1.09
6:B:1:OG6:HH21	6:B:1:OG6:HG31	1.20	1.06
2:B:129(A):ALA:HA	2:B:130:LEU:HD12	1.34	1.06
3:G:64:ASN:HA	3:G:67:ASN:HD22	1.15	1.06
2:B:41:LEU:HD12	2:B:42:CYS:N	1.71	1.06
2:B:138:VAL:HG22	2:B:199:PHE:HA	1.28	1.05
2:E:33:LEU:HD13	2:E:41:LEU:HD13	1.38	1.03
5:L:37:ASP:HA	5:L:40:LEU:HD12	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:SER:H	2:B:118:ILE:HB	1.21	1.02
2:B:192:GLU:HG2	2:B:220:CYS:SG	2.00	1.01
2:B:239:GLN:HA	2:B:242:ILE:HD11	1.42	1.01
2:B:70:LYS:HZ1	2:B:77:GLU:HG3	1.23	1.01
2:B:31:VAL:HB	2:B:44:ALA:HB3	1.42	1.01
2:B:99:LEU:HD12	6:B:1:OG6:HE2	1.42	1.01
2:B:238:ILE:O	2:B:241:VAL:HG22	1.63	0.98
2:B:45:SER:OG	2:B:53:LEU:HB3	1.62	0.98
2:B:176:ILE:HD13	2:B:176:ILE:H	1.28	0.97
5:L:2:VAL:HG13	5:L:3:ALA:H	1.28	0.95
2:E:123:LEU:HB2	2:E:235:LYS:HZ2	1.29	0.95
4:H:67:HIS:HB2	4:H:75:LEU:HD21	1.49	0.95
5:I:36:VAL:HG12	5:I:40:LEU:HD11	1.46	0.95
2:E:87:LYS:HD2	2:E:89:TYR:CE1	2.02	0.95
4:H:87:LEU:CD2	5:L:14:ARG:HH21	1.79	0.95
2:B:177:THR:HG22	2:B:179:ASN:H	1.30	0.94
2:E:163:VAL:HG23	2:E:183:ALA:HA	1.49	0.94
2:E:204(B):ASN:N	2:E:204(B):ASN:HD22	1.61	0.93
4:K:79:GLY:HA2	4:K:82:LEU:HD12	1.51	0.93
2:E:204(B):ASN:HD22	2:E:204(B):ASN:H	1.04	0.92
2:E:179:ASN:O	2:E:230:HIS:HB2	1.68	0.92
2:B:61:GLU:HG3	2:B:88:ILE:HG13	1.49	0.92
2:E:73:ARG:HE	2:E:74:THR:HG23	1.32	0.92
2:B:60(A):TYR:H	2:B:60(F):LYS:HB3	1.31	0.92
2:B:17:VAL:HG23	2:B:189:ASP:O	1.71	0.91
5:L:41:GLN:HA	5:L:44:GLU:OE2	1.70	0.91
4:H:89:GLN:O	4:H:93:ILE:HG12	1.71	0.91
2:B:62:ASN:H	2:B:62:ASN:ND2	1.65	0.91
1:A:12:LEU:HD23	1:A:13:GLU:N	1.85	0.90
2:E:127:GLU:O	2:E:129(B):SER:HB2	1.72	0.89
2:B:149(C):VAL:HG12	2:B:149(D):GLY:H	1.33	0.89
2:E:46:LEU:HA	2:E:52:VAL:HG22	1.53	0.89
2:B:33:LEU:HD23	2:B:34:PHE:N	1.88	0.89
2:E:60:LEU:HG	2:E:60(B):PRO:HD3	1.55	0.88
2:B:138:VAL:HG12	2:B:139:THR:H	1.37	0.88
5:I:10:ILE:HD12	5:I:10:ILE:H	1.39	0.88
4:H:104:VAL:HG12	4:H:105:GLU:HG3	1.56	0.88
2:E:231:VAL:HG13	2:E:232:PHE:H	1.39	0.88
2:E:212:ILE:HB	2:E:229:THR:HB	1.55	0.87
3:G:43:TYR:O	3:G:44:LYS:HG3	1.73	0.87
2:B:115:SER:N	2:B:118:ILE:HB	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:LEU:HD23	1:D:13:GLU:H	1.38	0.87
2:E:33:LEU:HA	2:E:66:VAL:HG12	1.56	0.87
2:E:123:LEU:HB2	2:E:235:LYS:NZ	1.88	0.87
2:B:142:GLY:HA3	2:B:194:ASP:OD2	1.76	0.86
4:K:67:HIS:CE1	4:K:72:LEU:HD13	2.11	0.86
2:E:99:LEU:HD11	6:E:1:OG6:CB1	2.05	0.85
2:E:138:VAL:CG2	2:E:199:PHE:HA	2.04	0.85
2:B:99:LEU:CD1	6:B:1:OG6:HE2	2.05	0.85
2:B:18:GLU:HG3	2:B:187:ARG:HB3	1.57	0.85
2:B:18:GLU:HB2	2:B:188:GLY:CA	2.07	0.85
2:E:68:ILE:HD12	2:E:68:ILE:H	1.41	0.85
2:E:60(A):TYR:N	2:E:60(F):LYS:HB3	1.92	0.85
2:E:57:HIS:HB3	2:E:102:ASP:OD1	1.77	0.84
4:H:86:LEU:HD11	5:I:25:ILE:HG23	1.58	0.84
2:E:26:MET:HE2	2:E:137:ARG:NH1	1.93	0.84
2:B:33:LEU:HD13	2:B:41:LEU:HD11	1.58	0.84
2:B:60(A):TYR:CE2	2:B:60(C):PRO:HB2	2.12	0.84
2:B:138:VAL:HG13	2:B:198:PRO:O	1.78	0.84
2:B:143:ASN:HD22	2:B:192:GLU:HB2	1.43	0.83
3:J:45:CYS:HB3	3:J:46:PRO:HD2	1.60	0.83
4:K:98:ASP:HA	4:K:101:ASN:ND2	1.92	0.83
5:I:36:VAL:O	5:I:40:LEU:HG	1.77	0.83
2:B:215:TRP:HA	6:B:1:OG6:HD22	1.59	0.83
2:B:110:LYS:HD2	3:J:39:GLU:OE2	1.79	0.83
2:B:135:LYS:HA	2:B:161:PRO:HA	1.58	0.83
2:B:144:LEU:O	2:B:145:LYS:HB3	1.77	0.83
2:B:215:TRP:HZ3	2:B:217:GLU:HG3	1.42	0.83
2:B:95:ASN:HD21	2:B:97(A):GLU:HB3	1.44	0.82
4:H:87:LEU:HD22	5:L:14:ARG:HH21	1.44	0.82
2:E:77:GLU:HB2	2:E:80:GLU:HB2	1.61	0.82
2:E:179:ASN:OD1	2:E:233:ARG:HB3	1.79	0.82
3:J:69:LEU:HD12	5:L:43:LEU:HD23	1.58	0.82
2:B:70:LYS:NZ	2:B:77:GLU:HG3	1.94	0.82
2:B:41:LEU:HD12	2:B:42:CYS:H	1.44	0.82
2:B:180:MET:HG2	2:B:227:PHE:HD2	1.45	0.82
2:B:126:ARG:O	2:B:129:ALA:HB3	1.80	0.82
2:B:138:VAL:HA	2:B:198:PRO:O	1.78	0.82
2:E:27:SER:HG	2:E:29:TRP:CD1	1.95	0.82
2:E:238:ILE:O	2:E:242:ILE:HG23	1.79	0.82
2:E:182:CYS:HA	2:E:226:GLY:O	1.78	0.82
3:J:45:CYS:HB3	3:J:46:PRO:CD	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:PRO:HB3	2:B:210:MET:HE1	1.60	0.81
5:I:37:ASP:HA	5:I:40:LEU:HD12	1.62	0.81
2:B:169:LYS:HG2	2:B:176:ILE:HG13	1.63	0.81
2:E:143:ASN:C	2:E:144:LEU:HD23	2.05	0.81
2:B:215:TRP:C	6:B:1:OG6:HE	1.88	0.81
2:E:33:LEU:HD22	2:E:41:LEU:HD11	1.62	0.81
4:H:69:ASP:HB3	4:H:72:LEU:HD12	1.63	0.81
4:K:89:GLN:O	4:K:93:ILE:HD13	1.79	0.81
3:J:62:PHE:HD2	5:L:36:VAL:HG11	1.44	0.81
4:K:66:LEU:O	4:K:66:LEU:HD23	1.80	0.80
1:D:4:ARG:HB2	1:D:7:PHE:HB2	1.62	0.80
2:B:202:LYS:HZ2	2:B:207:TRP:NE1	1.80	0.80
1:A:14(F):LEU:HD11	2:B:136:GLY:HA2	1.64	0.79
2:B:99:LEU:HD11	6:B:1:OG6:HB21	1.61	0.79
1:D:14(E):GLU:OE2	2:E:159:ASN:HB2	1.83	0.79
5:L:40:LEU:HB3	5:L:44:GLU:OE1	1.80	0.79
5:I:10:ILE:HA	5:I:17:SER:HA	1.65	0.79
2:B:60(A):TYR:N	2:B:60(F):LYS:HB3	1.97	0.79
2:E:134:TYR:O	2:E:162:ILE:HG13	1.82	0.79
2:B:232:PHE:HA	2:B:235:LYS:HB2	1.65	0.79
2:B:60:LEU:HA	2:B:60(F):LYS:O	1.83	0.79
3:G:49:CYS:H	4:H:76:CYS:HB3	1.47	0.78
5:I:35:LYS:O	5:I:39:ASP:OD2	2.01	0.78
2:B:65:LEU:HA	2:B:85:LEU:HD21	1.64	0.78
3:G:41:TRP:O	3:G:42:ASN:HB2	1.81	0.78
5:L:8:CYS:SG	5:L:10:ILE:HG13	2.23	0.78
2:E:62:ASN:HD22	2:E:62:ASN:H	1.32	0.78
2:E:179:ASN:ND2	2:E:233:ARG:HD3	1.98	0.78
2:E:204:PRO:HG2	2:E:204(A):PHE:H	1.49	0.78
2:E:46:LEU:HD22	2:E:47:ILE:N	1.99	0.78
2:B:35:ARG:O	2:B:38:GLN:HA	1.83	0.77
2:B:235:LYS:O	2:B:238:ILE:HB	1.84	0.77
5:I:11:LEU:HD22	5:L:2:VAL:O	1.85	0.77
2:B:91:HIS:ND1	2:B:92:PRO:HD2	2.00	0.77
2:E:134:TYR:HB2	2:E:162:ILE:HD12	1.65	0.77
4:K:67:HIS:CE1	4:K:69:ASP:H	2.03	0.77
2:B:214:SER:HG	2:B:215:TRP:HD1	1.33	0.77
4:H:97:VAL:O	4:H:101:ASN:ND2	2.18	0.76
2:B:18:GLU:HG3	2:B:188:GLY:N	2.00	0.76
2:B:144:LEU:CD2	2:B:152:PRO:HD3	2.14	0.76
4:H:87:LEU:HD21	5:L:14:ARG:HH21	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:65:ARG:HA	3:J:68:LYS:HD2	1.66	0.76
2:B:22:ALA:HB2	2:B:157:VAL:HG23	1.66	0.76
3:G:46:PRO:HD2	5:I:22:THR:HB	1.68	0.76
1:D:14(D):ARG:HH12	1:D:15:ARG:HD2	1.50	0.76
4:K:98:ASP:CA	4:K:101:ASN:HD21	1.96	0.76
1:A:12:LEU:CD2	1:A:13:GLU:H	1.96	0.76
2:E:182:CYS:HB2	2:E:225:TYR:HB2	1.67	0.75
2:E:126:ARG:O	2:E:129:ALA:HB3	1.86	0.75
2:B:131:GLN:O	2:B:162:ILE:HB	1.86	0.75
1:D:14(G):LEU:HD13	1:D:14(J):TYR:HE2	1.51	0.75
2:E:179:ASN:OD1	2:E:230:HIS:HB3	1.86	0.75
2:B:128:THR:O	2:B:129(C):LEU:HD13	1.86	0.75
1:D:11:SER:O	1:D:12:LEU:HB2	1.87	0.75
5:L:10:ILE:HD12	5:L:11:LEU:N	2.01	0.75
2:E:231:VAL:O	2:E:235:LYS:N	2.20	0.75
2:B:77(A):ARG:NH2	4:H:72:LEU:HD11	2.01	0.74
3:G:55:ILE:HD13	4:H:86:LEU:HD21	1.68	0.74
2:B:176:ILE:HD13	2:B:176:ILE:N	2.02	0.74
1:D:14(G):LEU:HA	1:D:14(J):TYR:CD2	2.22	0.74
2:B:68:ILE:HD12	2:B:68:ILE:N	2.01	0.74
2:B:124:PRO:HB3	2:B:210:MET:SD	2.27	0.74
2:B:135:LYS:HG2	2:B:161:PRO:N	2.02	0.74
2:B:185:LYS:H	2:B:185:LYS:HD2	1.52	0.74
4:H:101:ASN:O	4:H:105:GLU:HG3	1.87	0.74
3:J:62:PHE:HD1	3:J:62:PHE:H	1.35	0.74
5:I:28:PHE:HE1	5:L:14:ARG:HB3	1.51	0.74
2:B:146:GLU:HB2	2:B:149(B):ASN:ND2	2.02	0.74
1:D:14(G):LEU:HD13	1:D:14(J):TYR:CE2	2.23	0.74
2:E:70:LYS:HE3	2:E:72:SER:O	1.88	0.74
3:J:46:PRO:HB2	5:L:22:THR:HB	1.68	0.73
2:B:16:ILE:CD1	2:B:190:ALA:HA	2.18	0.73
2:E:171:SER:C	2:E:224:LYS:HZ3	1.95	0.73
2:B:55:ALA:H	2:B:196:GLY:HA2	1.53	0.73
3:G:62:PHE:O	3:G:66:ILE:HG12	1.88	0.73
2:B:51:TRP:CE2	2:B:242:ILE:HG22	2.23	0.73
2:B:138:VAL:HG12	2:B:139:THR:N	2.02	0.73
2:E:35:ARG:NH1	2:E:37:PRO:HD2	2.03	0.73
3:G:44:LYS:HA	4:K:76:CYS:O	1.88	0.73
3:J:63:THR:O	3:J:66:ILE:N	2.21	0.73
2:B:124:PRO:HB3	2:B:210:MET:CE	2.19	0.73
2:E:68:ILE:HD12	2:E:68:ILE:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:2:VAL:HG13	5:L:3:ALA:N	2.03	0.73
2:B:176:ILE:H	2:B:176:ILE:CD1	2.00	0.72
2:B:135:LYS:HE3	2:B:161:PRO:HD3	1.70	0.72
2:E:105:LEU:C	2:E:106:MET:HG3	2.11	0.72
5:I:11:LEU:HD13	5:L:2:VAL:HG23	1.71	0.72
6:B:1:0G6:HH21	6:B:1:0G6:CG2	1.98	0.72
4:H:86:LEU:HD12	5:L:15:PHE:HE2	1.52	0.72
2:E:145:LYS:C	2:E:146:GLU:OE2	2.32	0.72
2:E:142:GLY:HA3	2:E:194:ASP:CG	2.14	0.72
2:E:215:TRP:HB2	6:E:1:0G6:O	1.89	0.72
2:B:35:ARG:NH1	2:B:37:PRO:HD2	2.05	0.72
2:B:216:GLY:N	6:B:1:0G6:HE	1.86	0.72
2:B:53:LEU:HD21	2:B:212:ILE:HD11	1.72	0.72
2:E:200:VAL:HA	2:E:209:GLN:HA	1.70	0.72
2:B:133:GLY:N	2:B:162:ILE:O	2.23	0.71
2:E:138:VAL:HG13	2:E:198:PRO:C	2.14	0.71
2:B:38:GLN:H	2:B:38:GLN:CD	1.96	0.71
2:B:114:PHE:HA	2:B:118:ILE:CG2	2.19	0.71
2:B:129(A):ALA:CA	2:B:130:LEU:HD12	2.19	0.71
2:E:46:LEU:HD13	2:E:120:PRO:HA	1.71	0.71
4:H:101:ASN:ND2	4:H:101:ASN:N	2.36	0.71
5:I:11:LEU:HD13	5:L:2:VAL:CG2	2.20	0.71
5:L:8:CYS:SG	5:L:9:CYS:N	2.62	0.71
2:B:32:MET:HG2	2:B:40:LEU:HD13	1.70	0.71
1:D:12:LEU:HD23	1:D:13:GLU:N	2.06	0.71
2:B:30:GLN:OE1	2:B:139:THR:HB	1.89	0.71
2:B:191:CYS:HA	6:B:1:0G6:HH22	1.55	0.71
2:E:72:SER:HA	2:E:153:SER:O	1.90	0.71
3:G:58:VAL:HG13	3:G:62:PHE:CE1	2.26	0.71
2:B:50:ARG:HA	2:B:108:LEU:HB2	1.72	0.71
3:J:64:ASN:OD1	3:J:65:ARG:HG3	1.90	0.71
2:B:144:LEU:HD21	2:B:152:PRO:HD3	1.71	0.70
2:B:236:LYS:HB2	2:B:240:LYS:HZ1	1.55	0.70
2:E:169:LYS:HD2	2:E:176:ILE:HG21	1.74	0.70
2:B:51:TRP:HZ2	2:B:246:GLY:HA2	1.55	0.70
2:E:114:PHE:HA	2:E:118:ILE:HB	1.73	0.70
2:E:201:MET:N	2:E:208:TYR:O	2.24	0.70
1:A:14:ASP:H	1:A:14(C):GLU:HB2	1.57	0.70
2:B:71:HIS:O	2:B:154:VAL:HA	1.90	0.70
4:K:89:GLN:O	4:K:92:PRO:HG2	1.91	0.70
2:E:232:PHE:O	2:E:235:LYS:HB3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:11:LEU:HD21	5:L:3:ALA:HB2	1.73	0.70
2:E:145:LYS:NZ	2:E:147:THR:HA	2.06	0.70
2:E:239:GLN:O	2:E:242:ILE:HG12	1.92	0.70
3:J:62:PHE:CD2	5:L:36:VAL:HG11	2.25	0.70
1:A:6:LEU:HD12	1:A:6:LEU:H	1.56	0.69
2:E:138:VAL:HG13	2:E:198:PRO:O	1.92	0.69
2:E:158:VAL:O	2:E:158:VAL:HG13	1.92	0.69
2:B:137:ARG:HB3	2:B:200:VAL:CG2	2.22	0.69
2:E:204(B):ASN:N	2:E:204(B):ASN:ND2	2.31	0.69
4:K:69:ASP:HB3	4:K:72:LEU:CD1	2.21	0.69
1:D:14(D):ARG:HH12	1:D:15:ARG:CD	2.06	0.69
3:J:64:ASN:OD1	3:J:65:ARG:N	2.26	0.69
2:E:115:SER:H	2:E:118:ILE:HB	1.58	0.69
2:E:129:ALA:O	2:E:130:LEU:HG	1.93	0.69
2:B:66:VAL:HG23	2:B:68:ILE:HD11	1.74	0.69
2:B:98:ASN:O	2:B:180:MET:HE1	1.93	0.69
2:E:137:ARG:O	2:E:200:VAL:HG22	1.92	0.69
1:A:4:ARG:HE	1:A:8:GLU:CD	2.01	0.69
2:E:219:GLY:O	6:E:1:OG6:NH2	2.26	0.69
3:G:36:CYS:SG	4:K:75:LEU:HD12	2.33	0.69
4:H:87:LEU:HD22	5:L:14:ARG:NH2	2.07	0.69
5:I:9:CYS:O	5:I:11:LEU:HG	1.93	0.69
2:E:137:ARG:HA	2:E:158:VAL:O	1.93	0.69
2:E:139:THR:HG22	2:E:156:GLN:O	1.92	0.69
2:B:56:ALA:HB2	2:B:103:ILE:C	2.18	0.68
2:B:62:ASN:ND2	2:B:62:ASN:N	2.41	0.68
2:B:143:ASN:HD21	2:B:147:THR:HG22	1.57	0.68
6:B:1:OG6:HG31	6:B:1:OG6:NH2	1.91	0.68
2:E:60:LEU:HA	2:E:60(F):LYS:HG2	1.74	0.68
2:B:18:GLU:HB2	2:B:188:GLY:HA2	1.75	0.68
2:E:33:LEU:HD22	2:E:41:LEU:CD1	2.24	0.68
2:E:135:LYS:HA	2:E:161:PRO:HA	1.76	0.68
2:B:145:LYS:CD	2:B:149(B):ASN:HB3	2.23	0.68
1:D:14(G):LEU:HA	1:D:14(J):TYR:CE2	2.28	0.68
3:G:52:LYS:HD2	3:G:56:ASP:OD2	1.94	0.68
5:L:10:ILE:O	5:L:11:LEU:O	2.11	0.68
2:E:164:GLU:HG2	2:E:167:VAL:HG23	1.76	0.68
3:J:59:ASN:O	3:J:63:THR:HG23	1.94	0.68
2:E:168:CYS:O	2:E:172:THR:HG22	1.94	0.68
2:B:29:TRP:HA	2:B:46:LEU:HB3	1.76	0.67
3:G:64:ASN:CA	3:G:67:ASN:HD22	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:TYR:O	2:B:162:ILE:N	2.27	0.67
2:B:214:SER:OG	2:B:215:TRP:HD1	1.75	0.67
2:B:60(C):PRO:HD3	2:B:96:TRP:CZ3	2.30	0.67
2:E:31:VAL:HG22	2:E:46:LEU:HB2	1.76	0.67
2:E:146:GLU:O	2:E:149(B):ASN:ND2	2.26	0.67
3:G:63:THR:O	3:G:66:ILE:N	2.27	0.67
4:H:67:HIS:CB	4:H:75:LEU:HD21	2.23	0.67
2:B:33:LEU:HD22	2:B:41:LEU:HD11	1.75	0.67
4:K:78:THR:O	4:K:82:LEU:HG	1.95	0.67
2:B:143:ASN:ND2	2:B:147:THR:HG22	2.10	0.67
4:K:67:HIS:ND1	4:K:72:LEU:HB2	2.10	0.67
4:H:98:ASP:CA	4:H:101:ASN:HD21	2.07	0.67
2:B:138:VAL:HG13	2:B:198:PRO:C	2.19	0.67
2:E:138:VAL:O	2:E:158:VAL:HG12	1.94	0.67
5:I:8:CYS:O	5:L:8:CYS:HA	1.95	0.67
2:E:181:PHE:CZ	2:E:228:TYR:HB2	2.30	0.67
2:B:45:SER:HG	2:B:53:LEU:HB3	1.59	0.66
2:B:143:ASN:ND2	2:B:192:GLU:HB2	2.10	0.66
2:E:126:ARG:HA	2:E:232:PHE:CZ	2.30	0.66
2:B:46:LEU:HD22	2:B:120:PRO:HB3	1.76	0.66
2:E:33:LEU:O	2:E:41:LEU:HD12	1.95	0.66
2:E:79:ILE:HG23	2:E:117:TYR:CD2	2.30	0.66
2:B:33:LEU:HD23	2:B:33:LEU:C	2.20	0.66
2:E:87:LYS:HD3	2:E:88:ILE:O	1.94	0.66
2:B:86:GLU:HB2	2:B:109:LYS:HA	1.77	0.66
2:B:135:LYS:HG2	2:B:160:LEU:C	2.21	0.66
2:B:23:GLU:N	2:B:26:MET:HE3	2.10	0.66
2:E:38:GLN:CD	2:E:38:GLN:N	2.52	0.66
2:B:94:TYR:OH	2:B:96:TRP:HB3	1.96	0.66
2:B:100:ASP:OD1	2:B:101:ARG:HG3	1.96	0.66
2:E:145:LYS:HE3	2:E:147:THR:HG22	1.77	0.66
3:J:64:ASN:HA	3:J:67:ASN:ND2	2.11	0.66
4:K:67:HIS:ND1	4:K:72:LEU:HD13	2.11	0.66
4:K:76:CYS:HB3	4:K:77:PRO:CD	2.26	0.66
2:E:76:TYR:CE2	2:E:77(A):ARG:HG2	2.30	0.66
3:J:62:PHE:O	3:J:66:ILE:HD12	1.95	0.66
2:B:18:GLU:HG3	2:B:187:ARG:CB	2.26	0.65
5:I:41:GLN:HA	5:I:44:GLU:CD	2.21	0.65
2:B:32:MET:HE2	2:B:40:LEU:HD22	1.78	0.65
2:B:99:LEU:CD1	6:B:1:OG6:HB21	2.26	0.65
1:D:14:ASP:HB2	2:E:26:MET:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:138:VAL:HA	2:E:198:PRO:O	1.96	0.65
2:E:171:SER:O	2:E:224:LYS:NZ	2.22	0.65
2:E:202:LYS:HB2	2:E:207:TRP:CE3	2.32	0.65
2:B:137:ARG:O	2:B:200:VAL:HG22	1.96	0.65
2:E:124:PRO:HG2	2:E:235:LYS:CD	2.26	0.65
3:J:50:ARG:HG2	3:J:50:ARG:HH11	1.61	0.65
2:B:143:ASN:HB3	2:B:191:CYS:SG	2.36	0.65
2:E:60:LEU:HD12	2:E:60(F):LYS:O	1.96	0.65
2:E:182:CYS:O	2:E:183:ALA:HB2	1.97	0.65
5:I:19:CYS:HB3	5:I:20:PRO:CD	2.26	0.65
2:E:45:SER:HB2	2:E:53:LEU:HB3	1.78	0.65
3:G:50:ARG:HA	4:H:61:ASP:HA	1.78	0.65
2:B:145:LYS:CE	2:B:149(B):ASN:HB3	2.27	0.65
2:B:182:CYS:HB3	2:B:227:PHE:CE1	2.32	0.65
3:J:62:PHE:HD1	3:J:62:PHE:N	1.92	0.65
2:B:33:LEU:HD22	2:B:41:LEU:CG	2.27	0.65
4:H:101:ASN:HD22	4:H:101:ASN:H	1.45	0.65
2:B:23:GLU:H	2:B:26:MET:CE	2.11	0.64
2:B:50:ARG:NH1	2:B:111:PRO:HD3	2.13	0.64
2:B:73:ARG:NH1	2:B:151:GLN:HB3	2.12	0.64
2:B:184(A):TYR:OH	2:B:186(D):LYS:HE2	1.97	0.64
2:E:45:SER:O	2:E:52:VAL:HG13	1.97	0.64
2:E:71:HIS:O	2:E:154:VAL:HA	1.97	0.64
2:B:236:LYS:HG3	2:B:237:TRP:H	1.61	0.64
2:B:236:LYS:O	2:B:240:LYS:HG2	1.96	0.64
3:J:62:PHE:N	3:J:62:PHE:CD1	2.61	0.64
2:B:16:ILE:HD13	2:B:194:ASP:OD1	1.97	0.64
2:E:26:MET:HE2	2:E:137:ARG:CZ	2.27	0.64
4:H:67:HIS:HB2	4:H:75:LEU:CD2	2.24	0.64
3:J:33:TRP:CE3	3:J:33:TRP:HA	2.33	0.64
3:J:50:ARG:NH2	4:K:59:ALA:HB3	2.11	0.64
4:K:77:PRO:HB2	4:K:82:LEU:HD21	1.79	0.64
2:B:129(C):LEU:HD11	2:B:204(A):PHE:HE2	1.61	0.64
2:B:211:GLY:HA2	2:B:229:THR:O	1.98	0.64
2:B:236:LYS:HB2	2:B:240:LYS:NZ	2.11	0.64
1:A:4:ARG:H	1:A:8:GLU:CD	2.06	0.64
2:B:99:LEU:HB3	2:B:102:ASP:HB2	1.80	0.64
2:B:239:GLN:HA	2:B:242:ILE:CD1	2.21	0.64
2:E:45:SER:O	2:E:47:ILE:HD13	1.98	0.64
2:E:203:SER:N	2:E:206:ARG:O	2.24	0.64
1:A:11:SER:O	1:A:12:LEU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:220:CYS:HA	6:E:1:OG6:NH2	2.12	0.64
4:K:57:ARG:HH11	4:K:57:ARG:HG3	1.63	0.64
3:G:51:MET:HA	3:G:54:LEU:HD12	1.79	0.64
2:E:212:ILE:HB	2:E:229:THR:CB	2.27	0.64
3:G:58:VAL:HG12	3:G:59:ASN:N	2.12	0.64
5:I:37:ASP:HA	5:I:40:LEU:CD1	2.27	0.64
3:J:52:LYS:HE3	3:J:56:ASP:OD1	1.98	0.64
2:B:35:ARG:CZ	2:B:37:PRO:HD2	2.28	0.64
2:B:114:PHE:HA	2:B:118:ILE:HG22	1.78	0.64
2:B:138:VAL:HA	2:B:200:VAL:HG13	1.79	0.64
2:B:204(B):ASN:H	2:B:204(B):ASN:ND2	1.96	0.64
2:E:172:THR:HG21	2:E:176:ILE:HD11	1.80	0.64
1:A:1(C):GLU:O	1:A:1(B):ALA:HB3	1.98	0.64
3:G:49:CYS:N	4:H:76:CYS:HB3	2.12	0.64
2:E:134:TYR:HB2	2:E:162:ILE:CD1	2.27	0.63
2:B:33:LEU:HD22	2:B:41:LEU:HD21	1.79	0.63
3:J:49:CYS:N	4:K:76:CYS:HB3	2.14	0.63
2:B:100:ASP:O	2:B:101:ARG:HB2	1.97	0.63
2:E:202:LYS:HA	2:E:207:TRP:HA	1.80	0.63
1:A:4:ARG:NH2	2:B:207:TRP:HE1	1.95	0.63
1:A:12:LEU:CD2	1:A:13:GLU:N	2.58	0.63
2:B:63:ASP:N	2:B:63:ASP:OD2	2.29	0.63
2:E:46:LEU:HD13	2:E:120:PRO:CA	2.27	0.63
2:B:47:ILE:HA	2:B:120:PRO:HB2	1.80	0.63
2:E:142:GLY:CA	2:E:194:ASP:OD1	2.47	0.63
2:B:204(B):ASN:H	2:B:204(B):ASN:HD22	1.46	0.63
2:E:143:ASN:O	2:E:144:LEU:HD23	1.98	0.63
3:G:47:SER:O	3:G:48:GLY:C	2.41	0.63
2:B:214:SER:HG	2:B:215:TRP:CD1	2.16	0.63
1:D:13:GLU:HB3	1:D:14(C):GLU:HB2	1.80	0.63
4:K:78:THR:HG23	4:K:81:GLN:HG2	1.80	0.63
2:E:182:CYS:HB3	2:E:227:PHE:CE1	2.34	0.63
4:K:67:HIS:CE1	4:K:69:ASP:HB3	2.33	0.63
2:E:129(C):LEU:O	2:E:134:TYR:HD2	1.81	0.63
1:A:6:LEU:O	1:A:7:PHE:CD1	2.52	0.62
3:G:61:ASP:O	3:G:65:ARG:HB2	1.98	0.62
4:H:101:ASN:N	4:H:101:ASN:HD22	1.96	0.62
2:E:60(C):PRO:HG3	2:E:96:TRP:CZ3	2.34	0.62
2:E:204:PRO:HG2	2:E:204(A):PHE:CD2	2.34	0.62
2:E:216:GLY:HA3	6:E:1:OG6:NH1	2.14	0.62
2:E:51:TRP:HE3	2:E:105:LEU:HD22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:GLY:N	2:E:122:CYS:SG	2.71	0.62
2:E:32:MET:SD	2:E:70:LYS:HD3	2.38	0.62
4:K:78:THR:HG23	4:K:81:GLN:CG	2.29	0.62
2:B:137:ARG:HB3	2:B:200:VAL:HG22	1.80	0.62
2:B:95:ASN:HD21	2:B:97(A):GLU:CB	2.11	0.62
2:B:123:LEU:HB2	2:B:235:LYS:HE3	1.80	0.62
2:E:33:LEU:HD21	2:E:64:LEU:HB2	1.82	0.62
3:J:33:TRP:HA	3:J:33:TRP:HE3	1.63	0.62
1:A:4:ARG:HD2	2:B:26:MET:HA	1.81	0.62
1:A:13:GLU:HA	1:A:14(C):GLU:OE1	2.00	0.62
2:B:215:TRP:HB2	6:B:1:0G6:O	1.99	0.62
1:D:14(A):LYS:H	2:E:23:GLU:CD	2.07	0.62
2:E:90:ILE:HD11	2:E:94:TYR:CD2	2.35	0.62
3:G:51:MET:HA	3:G:54:LEU:CD1	2.30	0.62
3:J:63:THR:OG1	3:J:64:ASN:N	2.33	0.62
2:E:18:GLU:OE1	2:E:187:ARG:N	2.32	0.61
2:B:17:VAL:O	2:B:188:GLY:HA2	2.00	0.61
3:G:52:LYS:HG3	4:H:62:ALA:HB3	1.82	0.61
5:I:41:GLN:NE2	5:I:44:GLU:OE2	2.33	0.61
2:E:142:GLY:HA3	2:E:194:ASP:OD1	1.99	0.61
5:I:28:PHE:O	5:I:32:TYR:HB2	2.00	0.61
2:B:198:PRO:HA	2:B:209:GLN:CD	2.24	0.61
4:H:66:LEU:HD21	4:H:73:GLY:HA2	1.82	0.61
2:E:55:ALA:O	2:E:58:CYS:HB2	2.00	0.61
2:E:145:LYS:HZ2	2:E:147:THR:HA	1.65	0.61
3:G:45:CYS:HB2	5:I:22:THR:OG1	2.00	0.61
1:A:3:LEU:HD21	2:B:206:ARG:HG2	1.82	0.61
2:B:16:ILE:HG21	2:B:158:VAL:HB	1.82	0.61
2:B:72:SER:HA	2:B:153:SER:O	2.01	0.61
2:B:96:TRP:HA	2:B:99:LEU:HD23	1.82	0.61
2:E:138:VAL:O	2:E:139:THR:HG23	2.01	0.61
2:B:60(A):TYR:H	2:B:60(F):LYS:CB	2.09	0.61
2:E:73:ARG:HH21	2:E:74:THR:HG21	1.65	0.61
4:K:66:LEU:HD23	4:K:66:LEU:C	2.26	0.61
2:B:25:GLY:O	2:B:28:PRO:HD3	2.01	0.61
2:B:182:CYS:HB2	2:B:225:TYR:HB2	1.83	0.61
3:G:49:CYS:H	4:H:76:CYS:CB	2.13	0.61
3:J:29:LYS:O	3:J:29:LYS:HG3	2.01	0.61
2:B:142:GLY:HA3	2:B:194:ASP:CG	2.26	0.61
1:A:14:ASP:CG	1:A:14(C):GLU:HB2	2.26	0.60
5:L:37:ASP:O	5:L:40:LEU:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ILE:HD12	2:B:190:ALA:HA	1.82	0.60
2:B:76:TYR:HA	2:B:80:GLU:OE2	2.01	0.60
3:G:64:ASN:HA	3:G:67:ASN:ND2	2.01	0.60
2:E:29:TRP:HA	2:E:46:LEU:HB3	1.82	0.60
2:E:181:PHE:HE2	2:E:229:THR:O	1.85	0.60
5:I:35:LYS:O	5:I:38:LYS:HB3	2.00	0.60
5:L:31:THR:O	5:L:32:TYR:C	2.43	0.60
2:B:64:LEU:C	2:B:65:LEU:HD23	2.26	0.60
5:L:37:ASP:HA	5:L:40:LEU:CD1	2.24	0.60
1:A:6:LEU:CD2	2:B:25:GLY:HA3	2.31	0.60
1:A:14(H):GLU:HA	1:A:14(M):GLY:HA2	1.83	0.60
2:E:17:VAL:HG23	2:E:189:ASP:O	2.00	0.60
2:E:18:GLU:HB2	2:E:188:GLY:CA	2.32	0.60
2:E:204:PRO:HG2	2:E:204(A):PHE:N	2.16	0.60
2:B:30:GLN:HG2	2:B:155:LEU:HD22	1.83	0.60
2:B:137:ARG:C	2:B:200:VAL:HG22	2.26	0.60
2:B:184(A):TYR:CZ	2:B:186(D):LYS:HB2	2.36	0.60
2:E:54:THR:O	2:E:104:ALA:N	2.33	0.60
2:E:158:VAL:O	2:E:158:VAL:CG1	2.50	0.60
3:G:52:LYS:O	3:G:55:ILE:N	2.35	0.60
2:B:105:LEU:O	2:B:106:MET:HG3	2.01	0.60
2:B:99:LEU:HG	6:B:1:OG6:HZ	1.82	0.60
2:B:114:PHE:HA	2:B:118:ILE:HB	1.83	0.60
2:E:123:LEU:HD23	2:E:123:LEU:H	1.66	0.60
3:J:62:PHE:HE2	5:L:36:VAL:HB	1.67	0.60
2:E:47:ILE:O	2:E:48:SER:HB2	2.00	0.60
3:G:33:TRP:HE3	3:G:33:TRP:HA	1.67	0.60
2:B:137:ARG:O	2:B:200:VAL:N	2.35	0.59
2:B:191:CYS:SG	2:B:192:GLU:HG2	2.42	0.59
2:B:213:VAL:HA	2:B:228:TYR:HD2	1.66	0.59
2:E:163:VAL:CG2	2:E:183:ALA:HA	2.28	0.59
2:E:165:ARG:NH2	2:E:178:ASP:O	2.35	0.59
3:G:57:GLU:OE2	4:H:57:ARG:NH2	2.34	0.59
2:B:134:TYR:O	2:B:162:ILE:HG13	2.02	0.59
2:E:27:SER:OG	2:E:30:GLN:HB2	2.03	0.59
3:G:33:TRP:HA	3:G:33:TRP:CE3	2.37	0.59
3:J:29:LYS:O	3:J:30:ASP:C	2.45	0.59
2:B:23:GLU:H	2:B:26:MET:HE3	1.66	0.59
2:B:127:GLU:O	2:B:129(B):SER:HB2	2.02	0.59
5:I:32:TYR:O	5:I:36:VAL:HG23	2.03	0.59
5:I:39:ASP:O	5:I:43:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLY:HA3	2:B:199:PHE:HE1	1.67	0.59
2:B:136:GLY:N	2:B:160:LEU:O	2.32	0.59
2:E:70:LYS:HB2	2:E:141:TRP:CZ2	2.38	0.59
2:E:161:PRO:O	2:E:183:ALA:HB1	2.02	0.59
2:E:182:CYS:CB	2:E:225:TYR:HB2	2.33	0.59
2:E:213:VAL:HG22	2:E:228:TYR:CE2	2.36	0.59
2:B:78:ASN:N	2:B:78:ASN:HD22	1.98	0.59
2:E:131:GLN:O	2:E:134:TYR:HB2	2.03	0.59
2:B:61:GLU:OE1	2:B:61:GLU:N	2.35	0.59
2:B:244:GLN:HG3	2:B:245:PHE:CG	2.38	0.59
2:E:124:PRO:O	2:E:235:LYS:NZ	2.32	0.59
2:B:143:ASN:HB2	2:B:192:GLU:O	2.03	0.59
1:D:14:ASP:CG	2:E:137:ARG:HH22	2.11	0.59
2:E:99:LEU:HB2	6:E:1:OG6:HE2	1.84	0.59
2:E:137:ARG:HB3	2:E:200:VAL:CG2	2.33	0.59
2:E:228:TYR:N	2:E:228:TYR:CD1	2.71	0.59
2:E:35:ARG:O	2:E:37:PRO:O	2.20	0.59
2:E:95:ASN:OD1	2:E:97:ARG:HB2	2.02	0.59
3:J:50:ARG:HD2	3:J:54:LEU:HD11	1.85	0.59
2:B:62:ASN:H	2:B:62:ASN:HD22	1.45	0.58
2:B:129(C):LEU:N	2:B:129(C):LEU:HD12	2.18	0.58
2:B:132:ALA:HA	2:B:162:ILE:O	2.02	0.58
2:B:164:GLU:HG2	2:B:167:VAL:HG23	1.84	0.58
2:B:212:ILE:O	2:B:214:SER:N	2.35	0.58
2:B:115:SER:H	2:B:118:ILE:CB	2.05	0.58
3:G:65:ARG:HA	3:G:68:LYS:HD2	1.83	0.58
2:B:181:PHE:CE1	2:B:228:TYR:HB2	2.38	0.58
1:D:13:GLU:HB3	1:D:14(C):GLU:CB	2.33	0.58
2:E:49:ASP:O	2:E:111:PRO:HA	2.03	0.58
2:E:103:ILE:HG12	2:E:104:ALA:N	2.18	0.58
5:I:28:PHE:CE1	5:L:14:ARG:HB3	2.37	0.58
2:E:60:LEU:HA	2:E:60(F):LYS:O	2.03	0.58
5:I:21:THR:O	5:I:25:ILE:HG12	2.03	0.58
3:J:32:ASP:O	3:J:33:TRP:CE3	2.57	0.58
4:K:82:LEU:O	4:K:85:ALA:HB3	2.04	0.58
1:A:14(D):ARG:O	1:A:14(H):GLU:HG2	2.04	0.58
2:B:61:GLU:HG3	2:B:88:ILE:CG1	2.27	0.58
1:D:14(C):GLU:O	1:D:14(G):LEU:HD23	2.02	0.58
2:E:124:PRO:HB3	2:E:210:MET:SD	2.44	0.58
2:E:182:CYS:CA	2:E:226:GLY:O	2.52	0.58
3:J:52:LYS:HG3	4:K:62:ALA:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:CYS:O	2:B:183:ALA:HB2	2.02	0.58
2:E:138:VAL:HG22	2:E:199:PHE:CA	2.17	0.58
2:E:182:CYS:HA	2:E:227:PHE:HA	1.85	0.58
2:B:135:LYS:HE2	2:B:160:LEU:HA	1.84	0.58
2:B:165:ARG:C	2:B:169:LYS:HD3	2.28	0.58
2:E:201:MET:O	2:E:208:TYR:N	2.36	0.58
3:G:51:MET:O	3:G:55:ILE:HG13	2.02	0.58
4:K:69:ASP:HB3	4:K:72:LEU:HD13	1.85	0.58
2:B:82:ILE:HB	3:J:38:ASP:OD1	2.04	0.58
2:B:191:CYS:HA	6:B:1:0G6:NH2	2.19	0.58
2:B:215:TRP:CB	6:B:1:0G6:HA1	2.33	0.58
2:E:203:SER:OG	2:E:204(B):ASN:ND2	2.36	0.58
3:G:64:ASN:OD1	3:G:65:ARG:N	2.36	0.58
4:H:98:ASP:O	4:H:101:ASN:OD1	2.21	0.58
3:J:50:ARG:HH21	4:K:59:ALA:HB3	1.68	0.58
2:B:145:LYS:HD2	2:B:149(B):ASN:HB3	1.85	0.58
2:E:55:ALA:HB3	2:E:58:CYS:SG	2.43	0.58
2:B:32:MET:HB3	2:B:67:ARG:HB2	1.86	0.58
2:B:32:MET:HE1	2:B:73:ARG:O	2.03	0.58
2:B:59:LEU:O	2:B:60(F):LYS:HG2	2.04	0.58
2:B:145:LYS:HE3	2:B:149(B):ASN:HB3	1.84	0.58
4:H:65:CYS:SG	4:H:65:CYS:O	2.61	0.58
5:I:40:LEU:N	5:I:40:LEU:HD23	2.19	0.58
2:B:33:LEU:CD1	2:B:41:LEU:HD11	2.30	0.57
2:B:124:PRO:HA	2:B:208:TYR:CE1	2.39	0.57
2:E:105:LEU:CD1	2:E:238:ILE:HG23	2.34	0.57
3:J:46:PRO:HB2	5:L:22:THR:CB	2.33	0.57
5:L:37:ASP:HA	5:L:40:LEU:HB2	1.86	0.57
2:B:57:HIS:CE1	6:B:1:0G6:HB31	2.39	0.57
2:E:129(C):LEU:O	2:E:134:TYR:CD2	2.57	0.57
5:L:37:ASP:CA	5:L:40:LEU:HD12	2.25	0.57
1:A:6:LEU:HD22	2:B:25:GLY:HA3	1.86	0.57
1:D:1:CYS:C	2:E:122:CYS:SG	2.87	0.57
4:H:100:LEU:O	4:H:102:ASN:N	2.37	0.57
2:E:191:CYS:HA	6:E:1:0G6:NH2	2.19	0.57
2:B:33:LEU:HD22	2:B:41:LEU:CD1	2.35	0.57
2:B:67:ARG:HG2	2:B:82:ILE:HG12	1.86	0.57
2:E:210:MET:HA	2:E:231:VAL:HG11	1.86	0.57
2:E:213:VAL:HA	2:E:228:TYR:CD2	2.38	0.57
2:B:51:TRP:CZ3	2:B:107:LYS:HB2	2.39	0.57
2:B:60(B):PRO:HA	2:B:60(E):ASP:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LEU:HD12	2:B:64:LEU:H	1.69	0.57
2:B:128:THR:HG22	2:B:129(C):LEU:HD22	1.85	0.57
1:A:4:ARG:N	1:A:8:GLU:OE1	2.33	0.57
2:B:46:LEU:CD2	2:B:48:SER:H	2.16	0.57
2:E:68:ILE:H	2:E:68:ILE:CD1	2.12	0.57
5:I:12:ASP:HB3	5:I:18:TYR:OH	2.05	0.57
5:I:41:GLN:O	5:I:45:ASP:OD2	2.22	0.57
2:B:29:TRP:CA	2:B:46:LEU:HB3	2.35	0.57
2:B:43:GLY:O	2:B:196:GLY:HA3	2.04	0.57
2:E:34:PHE:CD1	2:E:40:LEU:HA	2.40	0.57
2:E:182:CYS:SG	2:E:225:TYR:HB2	2.44	0.57
4:H:56:GLU:O	4:H:57:ARG:HB2	2.05	0.57
4:H:98:ASP:HA	4:H:101:ASN:HD21	1.70	0.57
2:B:22:ALA:CB	2:B:157:VAL:HG23	2.33	0.57
2:B:29:TRP:HB3	2:B:120:PRO:HA	1.87	0.57
2:B:70:LYS:O	2:B:141:TRP:HZ2	1.87	0.57
2:B:86:GLU:OE1	2:B:86:GLU:HA	2.03	0.57
2:E:87:LYS:HD2	2:E:89:TYR:CZ	2.40	0.57
2:E:90:ILE:HD13	2:E:91:HIS:N	2.20	0.57
2:E:198:PRO:O	2:E:198:PRO:HG2	2.04	0.57
5:I:21:THR:HG1	5:I:24:GLY:H	1.52	0.57
2:B:137:ARG:HA	2:B:158:VAL:O	2.04	0.56
2:B:143:ASN:C	2:B:144:LEU:HD23	2.30	0.56
2:B:147:THR:HG23	2:B:192:GLU:HG3	1.86	0.56
2:E:60(A):TYR:CE2	2:E:60(C):PRO:HB2	2.39	0.56
4:H:82:LEU:O	4:H:86:LEU:HG	2.05	0.56
2:B:47:ILE:HG22	2:B:121:VAL:HG13	1.86	0.56
2:B:31:VAL:HG12	2:B:66:VAL:HB	1.86	0.56
2:B:146:GLU:HB2	2:B:149(B):ASN:HD21	1.68	0.56
2:E:51:TRP:HE1	2:E:246:GLY:HA3	1.70	0.56
4:H:87:LEU:HD11	5:L:12:ASP:OD1	2.04	0.56
3:J:40:ASP:O	3:J:43:TYR:HB2	2.06	0.56
1:A:13:GLU:HB2	1:A:14(C):GLU:HB3	1.87	0.56
2:B:215:TRP:CE3	6:B:1:OG6:HB3	2.40	0.56
2:E:60(A):TYR:H	2:E:60(F):LYS:CB	1.99	0.56
2:B:215:TRP:CZ3	2:B:217:GLU:HG3	2.32	0.56
1:D:4:ARG:HE	1:D:8:GLU:CD	2.14	0.56
2:E:185:LYS:HB2	2:E:186(B):GLU:OE1	2.05	0.56
4:H:66:LEU:HA	4:H:74:VAL:HA	1.87	0.56
2:B:60(C):PRO:HD3	2:B:96:TRP:CE3	2.40	0.56
2:B:141:TRP:O	2:B:142:GLY:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:110:LYS:HG3	2:E:111:PRO:HD2	1.86	0.56
2:E:169:LYS:HA	2:E:176:ILE:HG13	1.88	0.56
3:G:51:MET:O	3:G:52:LYS:C	2.48	0.56
2:B:28:PRO:O	2:B:119:HIS:O	2.24	0.56
2:B:165:ARG:O	2:B:168:CYS:HB2	2.06	0.56
2:E:123:LEU:O	2:E:208:TYR:HE2	1.89	0.56
2:E:204(B):ASN:O	2:E:205:ASN:OD1	2.23	0.56
4:H:80:CYS:N	5:I:20:PRO:HD2	2.21	0.56
2:B:50:ARG:O	2:B:107:LYS:HA	2.05	0.56
2:B:98:ASN:O	2:B:99:LEU:HB2	2.05	0.56
5:I:11:LEU:HD12	5:I:18:TYR:CG	2.40	0.56
5:I:21:THR:OG1	5:I:23:CYS:HB2	2.05	0.56
2:B:213:VAL:HA	2:B:228:TYR:CD2	2.41	0.56
1:A:14(G):LEU:HA	1:A:14(J):TYR:CD2	2.40	0.55
2:B:203:SER:OG	2:B:204(A):PHE:HB2	2.05	0.55
2:B:215:TRP:CB	6:B:1:0G6:HD2	2.36	0.55
2:B:60(I):THR:HB	2:B:61:GLU:OE1	2.07	0.55
2:B:61:GLU:OE1	2:B:62:ASN:ND2	2.40	0.55
2:E:85:LEU:HA	2:E:109:LYS:H	1.70	0.55
2:E:137:ARG:HB3	2:E:200:VAL:HG22	1.89	0.55
4:H:98:ASP:C	4:H:101:ASN:HD21	2.13	0.55
1:A:5:PRO:HA	1:A:9:LYS:CB	2.37	0.55
4:H:101:ASN:O	4:H:104:VAL:HG12	2.07	0.55
4:K:83:GLN:O	4:K:86:LEU:HB2	2.07	0.55
2:E:60(F):LYS:HG3	2:E:60(H):PHE:CD2	2.42	0.55
3:J:51:MET:O	3:J:52:LYS:C	2.49	0.55
5:L:9:CYS:SG	5:L:10:ILE:HG23	2.46	0.55
2:B:46:LEU:HD22	2:B:47:ILE:N	2.22	0.55
2:B:185:LYS:H	2:B:185:LYS:CD	2.20	0.55
2:B:215:TRP:HB2	6:B:1:0G6:HD2	1.88	0.55
3:G:59:ASN:O	3:G:62:PHE:HB2	2.06	0.55
2:B:60(A):TYR:CZ	2:B:60(C):PRO:HG2	2.42	0.55
2:B:191:CYS:SG	2:B:192:GLU:N	2.79	0.55
2:E:20:SER:O	2:E:22:ALA:N	2.39	0.55
2:E:23:GLU:OE1	2:E:26:MET:HE3	2.07	0.55
2:E:51:TRP:HA	2:E:106:MET:O	2.07	0.55
4:K:76:CYS:HB3	4:K:77:PRO:HD2	1.88	0.55
2:B:105:LEU:C	2:B:106:MET:HG3	2.32	0.55
2:B:195:SER:C	2:B:197:GLY:H	2.13	0.55
1:D:14(I):SER:CB	2:E:135:LYS:HB2	2.36	0.55
2:E:151:GLN:HB3	2:E:152:PRO:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:GLN:HG3	2:B:245:PHE:CD1	2.42	0.55
4:K:69:ASP:HB3	4:K:72:LEU:HD12	1.89	0.55
2:B:61:GLU:CG	2:B:88:ILE:HG13	2.31	0.55
2:B:215:TRP:CE3	2:B:216:GLY:N	2.75	0.55
2:E:219:GLY:HA3	2:E:221:ARG:NH1	2.22	0.55
4:H:80:CYS:H	5:I:19:CYS:HB3	1.72	0.55
1:A:4:ARG:NH2	2:B:207:TRP:NE1	2.55	0.54
2:B:60(B):PRO:C	2:B:60(E):ASP:H	2.15	0.54
2:B:114:PHE:HA	2:B:118:ILE:CB	2.36	0.54
2:B:162:ILE:HD11	2:B:201:MET:HE3	1.89	0.54
2:E:62:ASN:H	2:E:62:ASN:ND2	2.01	0.54
2:E:127:GLU:O	2:E:128:THR:C	2.48	0.54
2:E:130:LEU:HD23	2:E:201:MET:HE1	1.89	0.54
2:B:138:VAL:CG1	2:B:139:THR:H	2.16	0.54
2:B:239:GLN:O	2:B:242:ILE:HG13	2.08	0.54
3:J:69:LEU:HD11	5:L:44:GLU:HA	1.89	0.54
2:B:60(D):TRP:CH2	6:B:1:0G6:HD21	2.42	0.54
1:D:4:ARG:CB	1:D:7:PHE:HB2	2.37	0.54
2:E:192:GLU:HA	6:E:1:0G6:HG31	1.89	0.54
3:J:37:SER:O	3:J:40:ASP:HB2	2.07	0.54
1:A:4:ARG:HH21	2:B:207:TRP:HE1	1.56	0.54
2:B:186(C):GLY:O	2:B:186(D):LYS:HG2	2.08	0.54
2:E:199:PHE:O	2:E:210:MET:N	2.41	0.54
2:E:232:PHE:O	2:E:235:LYS:CB	2.55	0.54
2:E:75:ARG:HG3	2:E:75:ARG:O	2.07	0.54
2:B:46:LEU:HD13	2:B:120:PRO:N	2.23	0.54
2:B:231:VAL:O	2:B:235:LYS:N	2.40	0.54
3:G:61:ASP:HA	3:G:64:ASN:ND2	2.22	0.54
4:H:98:ASP:HA	4:H:101:ASN:ND2	2.23	0.54
3:J:45:CYS:CB	3:J:46:PRO:CD	2.78	0.54
2:B:57:HIS:CD2	6:B:1:0G6:HB31	2.42	0.54
2:B:99:LEU:CD1	6:B:1:0G6:CE2	2.83	0.54
2:E:134:TYR:O	2:E:161:PRO:HA	2.08	0.54
2:E:231:VAL:HG13	2:E:232:PHE:N	2.17	0.54
4:H:93:ILE:HG22	4:H:94:ARG:N	2.21	0.54
2:B:163:VAL:HG11	2:B:167:VAL:HB	1.89	0.54
2:E:35:ARG:NE	2:E:36(A):SER:O	2.40	0.54
2:E:99:LEU:HD22	2:E:102:ASP:HB2	1.90	0.54
1:A:4:ARG:CD	2:B:26:MET:HA	2.38	0.54
2:B:71:HIS:C	2:B:154:VAL:HG22	2.33	0.54
2:B:73:ARG:HB2	2:B:141:TRP:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ALA:O	2:B:118:ILE:HG21	2.07	0.54
2:B:143:ASN:HD22	2:B:192:GLU:CB	2.16	0.54
2:B:192:GLU:CG	2:B:220:CYS:SG	2.87	0.54
2:B:237:TRP:HA	2:B:240:LYS:HG3	1.89	0.54
2:E:70:LYS:NZ	2:E:77:GLU:HG3	2.21	0.54
2:E:103:ILE:CD1	2:E:237:TRP:HZ3	2.21	0.54
2:E:107:LYS:NZ	2:E:246:GLY:HA2	2.23	0.54
2:E:124:PRO:HG2	2:E:235:LYS:HD2	1.89	0.54
2:E:145:LYS:HE3	2:E:147:THR:CG2	2.38	0.54
4:K:69:ASP:OD2	4:K:70:PRO:HD2	2.07	0.54
5:L:41:GLN:O	5:L:44:GLU:HB2	2.08	0.54
1:A:4:ARG:HD2	1:A:7:PHE:HD2	1.72	0.54
2:B:139:THR:O	2:B:198:PRO:HD2	2.07	0.54
4:H:90:GLU:HA	5:I:32:TYR:HH	1.73	0.54
3:J:49:CYS:H	4:K:76:CYS:CB	2.21	0.54
3:J:32:ASP:O	3:J:33:TRP:HE3	1.90	0.53
2:B:99:LEU:HG	6:B:1:OG6:CZ	2.38	0.53
2:B:143:ASN:O	2:B:144:LEU:HD23	2.07	0.53
2:B:202:LYS:NZ	2:B:207:TRP:NE1	2.53	0.53
2:E:32:MET:O	2:E:66:VAL:HA	2.09	0.53
2:E:203:SER:CB	2:E:204(B):ASN:HD21	2.20	0.53
5:L:25:ILE:O	5:L:26:ALA:C	2.50	0.53
2:E:99:LEU:HB3	2:E:102:ASP:HB2	1.90	0.53
2:E:204:PRO:HG2	2:E:204(A):PHE:HD2	1.71	0.53
3:G:35:PHE:CE2	4:K:68:ALA:HA	2.43	0.53
2:B:161:PRO:HG2	2:B:184:GLY:O	2.08	0.53
2:E:61:GLU:HG3	2:E:88:ILE:HG13	1.91	0.53
2:B:137:ARG:HG2	2:B:138:VAL:N	2.22	0.53
2:E:177:THR:HB	2:E:180:MET:H	1.74	0.53
2:E:220:CYS:HA	6:E:1:OG6:HH22	1.74	0.53
2:B:239:GLN:NE2	2:B:240:LYS:HE3	2.23	0.53
2:E:123:LEU:HD23	2:E:123:LEU:N	2.23	0.53
2:B:33:LEU:HD22	2:B:41:LEU:CD2	2.38	0.53
2:B:44:ALA:HB1	2:B:52:VAL:CG1	2.39	0.53
2:E:144:LEU:O	2:E:145:LYS:HB3	2.09	0.53
5:L:37:ASP:O	5:L:38:LYS:C	2.52	0.53
2:B:235:LYS:HA	2:B:238:ILE:HD12	1.91	0.53
2:E:35:ARG:HH11	2:E:37:PRO:HD2	1.73	0.53
2:E:137:ARG:C	2:E:200:VAL:HG22	2.33	0.53
2:E:182:CYS:O	2:E:183:ALA:CB	2.56	0.53
2:E:204:PRO:CG	2:E:204(A):PHE:H	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PRO:HA	1:A:9:LYS:HB3	1.91	0.53
2:B:60(B):PRO:O	2:B:60(E):ASP:N	2.34	0.53
2:E:131:GLN:O	2:E:162:ILE:HD12	2.09	0.53
4:H:71:ASP:O	3:J:50:ARG:NH1	2.42	0.53
2:B:172:THR:HG21	2:B:176:ILE:HG23	1.91	0.52
2:E:34:PHE:HE1	2:E:40:LEU:HB2	1.73	0.52
2:E:80:GLU:O	2:E:81:LYS:HD3	2.09	0.52
1:D:14(H):GLU:OE2	1:D:15:ARG:HB3	2.09	0.52
3:J:61:ASP:HA	3:J:64:ASN:HD21	1.73	0.52
2:B:27:SER:HB3	2:B:30:GLN:HB2	1.92	0.52
2:E:45:SER:HB2	2:E:53:LEU:CB	2.39	0.52
4:H:93:ILE:HG13	5:I:32:TYR:OH	2.09	0.52
1:A:14(K):ILE:H	2:B:134:TYR:HE1	1.57	0.52
2:B:58:CYS:O	2:B:60(F):LYS:HD3	2.09	0.52
2:B:135:LYS:HA	2:B:161:PRO:CA	2.34	0.52
3:G:64:ASN:O	3:G:67:ASN:HB2	2.09	0.52
4:H:67:HIS:HB2	4:H:75:LEU:HD11	1.91	0.52
2:B:78:ASN:C	2:B:79:ILE:HD12	2.34	0.52
2:B:144:LEU:HG	2:B:150:GLY:O	2.09	0.52
2:B:177:THR:HG22	2:B:178:ASP:N	2.24	0.52
2:E:129(B):SER:O	2:E:131:GLN:NE2	2.42	0.52
4:H:75:LEU:HB2	3:J:44:LYS:HB3	1.92	0.52
2:B:46:LEU:HD22	2:B:48:SER:H	1.74	0.52
2:E:57:HIS:CD2	6:E:1:OG6:HB31	2.44	0.52
2:E:66:VAL:HG22	2:E:85:LEU:HD21	1.91	0.52
2:B:23:GLU:HB2	2:B:26:MET:CE	2.40	0.52
2:B:50:ARG:HH12	2:B:111:PRO:HD3	1.72	0.52
2:B:122:CYS:HB3	2:B:208:TYR:HE2	1.75	0.52
2:B:149(C):VAL:HG12	2:B:149(D):GLY:N	2.13	0.52
2:E:236:LYS:O	2:E:237:TRP:C	2.53	0.52
2:B:68:ILE:HD12	2:B:68:ILE:H	1.70	0.52
2:B:154:VAL:O	2:B:155:LEU:C	2.52	0.52
5:I:11:LEU:HD12	5:I:18:TYR:CD2	2.44	0.52
3:J:59:ASN:O	3:J:62:PHE:HB2	2.10	0.52
2:B:146:GLU:H	2:B:149(B):ASN:ND2	2.08	0.52
2:E:232:PHE:HA	2:E:235:LYS:HB2	1.91	0.52
3:G:45:CYS:HB3	3:G:46:PRO:HD2	1.90	0.52
3:J:50:ARG:NH2	4:K:59:ALA:CB	2.73	0.52
2:B:33:LEU:HD21	2:B:64:LEU:HD22	1.91	0.52
2:B:101:ARG:O	2:B:103:ILE:HG22	2.10	0.52
2:E:57:HIS:CE1	6:E:1:OG6:H1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:163:VAL:HG13	2:E:185:LYS:NZ	2.25	0.52
2:E:56:ALA:HB2	2:E:103:ILE:O	2.10	0.51
3:G:50:ARG:HD2	3:G:54:LEU:HD21	1.92	0.51
3:J:58:VAL:O	3:J:62:PHE:CD1	2.63	0.51
1:A:4:ARG:HD2	1:A:7:PHE:CD2	2.45	0.51
2:B:72:SER:OG	2:B:77:GLU:OE2	2.27	0.51
2:E:28:PRO:HD2	2:E:29:TRP:CE2	2.45	0.51
2:E:46:LEU:HD22	2:E:46:LEU:C	2.31	0.51
2:E:49:ASP:HB3	2:E:114:PHE:CE1	2.45	0.51
2:E:127:GLU:C	2:E:129(B):SER:HB2	2.35	0.51
5:I:11:LEU:CD2	5:L:3:ALA:HB2	2.40	0.51
5:L:40:LEU:O	5:L:41:GLN:C	2.52	0.51
2:B:198:PRO:O	2:B:198:PRO:HG2	2.09	0.51
2:E:202:LYS:HB2	2:E:207:TRP:CD2	2.45	0.51
3:G:62:PHE:HZ	5:I:33:GLN:HG2	1.75	0.51
3:J:51:MET:O	3:J:55:ILE:HD12	2.11	0.51
3:J:58:VAL:HG12	3:J:59:ASN:N	2.25	0.51
2:B:71:HIS:N	2:B:77:GLU:OE1	2.43	0.51
2:B:132:ALA:O	2:B:134:TYR:N	2.42	0.51
5:I:41:GLN:HA	5:I:44:GLU:OE2	2.10	0.51
3:J:61:ASP:HA	3:J:64:ASN:ND2	2.25	0.51
4:K:100:LEU:O	4:K:104:VAL:HG23	2.11	0.51
2:B:46:LEU:HD22	2:B:46:LEU:C	2.36	0.51
2:B:68:ILE:N	2:B:68:ILE:CD1	2.70	0.51
2:B:79:ILE:HD12	2:B:79:ILE:N	2.25	0.51
2:E:66:VAL:O	2:E:82:ILE:HG23	2.11	0.51
2:E:213:VAL:HG22	2:E:228:TYR:HE2	1.76	0.51
2:E:67:ARG:HA	2:E:82:ILE:HG12	1.92	0.51
2:E:90:ILE:HD11	2:E:94:TYR:HB3	1.92	0.51
2:E:164:GLU:HG2	2:E:167:VAL:CG2	2.40	0.51
5:L:11:LEU:HD12	5:L:18:TYR:CE1	2.45	0.51
5:L:28:PHE:O	5:L:32:TYR:CB	2.59	0.51
2:B:18:GLU:CG	2:B:188:GLY:N	2.74	0.51
2:B:203:SER:O	2:B:205:ASN:HA	2.11	0.51
2:E:46:LEU:HD22	2:E:48:SER:H	1.74	0.51
2:E:47:ILE:HA	2:E:120:PRO:HB2	1.93	0.51
2:E:129:ALA:HB1	2:E:232:PHE:CD2	2.46	0.51
2:E:191:CYS:HA	6:E:1:OG6:CZ1	2.40	0.51
4:H:78:THR:H	4:H:81:GLN:HB2	1.76	0.51
2:B:127:GLU:O	2:B:129:ALA:N	2.44	0.51
2:B:129(C):LEU:N	2:B:129(C):LEU:CD1	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14(H):GLU:HA	1:D:14(M):GLY:HA2	1.92	0.51
2:E:105:LEU:HD13	2:E:241:VAL:HG21	1.93	0.51
2:E:208:TYR:HB3	2:E:210:MET:SD	2.51	0.51
3:J:65:ARG:CA	3:J:68:LYS:HD2	2.38	0.51
1:A:1:CYS:O	1:A:3:LEU:N	2.44	0.51
2:B:33:LEU:C	2:B:33:LEU:CD2	2.84	0.51
2:B:202:LYS:HZ2	2:B:207:TRP:CD1	2.28	0.51
2:B:244:GLN:OE1	2:B:245:PHE:CE1	2.64	0.51
2:E:202:LYS:HB2	2:E:207:TRP:CZ3	2.45	0.51
4:H:66:LEU:CD2	4:H:73:GLY:HA2	2.40	0.51
1:D:1(C):GLU:C	1:D:1(A):ASP:N	2.68	0.50
1:D:4:ARG:HD2	1:D:7:PHE:CD2	2.46	0.50
2:E:76:TYR:CD2	2:E:77(A):ARG:HG2	2.45	0.50
2:E:154:VAL:O	2:E:155:LEU:C	2.54	0.50
2:E:238:ILE:O	2:E:241:VAL:HG13	2.11	0.50
3:J:49:CYS:H	4:K:76:CYS:HB3	1.76	0.50
2:B:86:GLU:HB2	2:B:109:LYS:CA	2.39	0.50
1:D:14(A):LYS:N	2:E:23:GLU:OE2	2.39	0.50
2:E:44:ALA:HB1	2:E:52:VAL:HG11	1.94	0.50
3:G:40:ASP:O	3:G:41:TRP:C	2.54	0.50
4:H:100:LEU:O	4:H:101:ASN:C	2.54	0.50
3:J:40:ASP:O	3:J:41:TRP:C	2.51	0.50
3:J:52:LYS:HA	3:J:55:ILE:HD13	1.93	0.50
4:K:67:HIS:HB2	4:K:75:LEU:HD11	1.92	0.50
2:B:77:GLU:HB2	2:B:80:GLU:HB3	1.93	0.50
2:E:32:MET:HG3	2:E:40:LEU:HD11	1.94	0.50
2:E:60(B):PRO:HB2	2:E:60(C):PRO:HD3	1.94	0.50
2:E:177:THR:HG22	2:E:178:ASP:H	1.75	0.50
4:H:89:GLN:O	4:H:93:ILE:CG1	2.52	0.50
5:I:11:LEU:HD13	5:L:2:VAL:HG22	1.94	0.50
4:K:82:LEU:O	4:K:83:GLN:C	2.55	0.50
1:A:2:GLY:C	1:A:3:LEU:HG	2.37	0.50
2:B:76:TYR:CE2	2:B:77(A):ARG:HA	2.46	0.50
2:B:212:ILE:O	2:B:213:VAL:C	2.54	0.50
3:J:58:VAL:HG13	3:J:62:PHE:CZ	2.46	0.50
2:B:18:GLU:OE1	2:B:187:ARG:HB2	2.12	0.50
2:B:128:THR:CG2	2:B:129(C):LEU:HD13	2.41	0.50
1:D:7:PHE:O	1:D:11:SER:N	2.44	0.50
2:E:50:ARG:O	2:E:107:LYS:HA	2.10	0.50
2:E:67:ARG:NE	2:E:70:LYS:HD2	2.26	0.50
3:G:64:ASN:OD1	3:G:65:ARG:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:12:ASP:O	5:I:15:PHE:N	2.42	0.50
1:A:14:ASP:OD1	1:A:14(C):GLU:N	2.45	0.50
2:B:115:SER:OG	2:B:118:ILE:HG12	2.11	0.50
2:E:105:LEU:HD13	2:E:241:VAL:CG2	2.42	0.50
2:E:203:SER:O	2:E:205:ASN:HA	2.11	0.50
3:G:51:MET:HG3	5:I:22:THR:HG22	1.93	0.50
2:B:146:GLU:CB	2:B:149(B):ASN:ND2	2.73	0.50
2:E:46:LEU:HD21	2:E:48:SER:O	2.11	0.50
2:E:67:ARG:HH21	2:E:80:GLU:CD	2.19	0.50
2:E:96:TRP:O	2:E:97:ARG:C	2.54	0.50
2:E:212:ILE:O	2:E:214:SER:N	2.44	0.50
3:J:62:PHE:CE2	5:L:36:VAL:HB	2.46	0.50
4:K:93:ILE:HG22	4:K:94:ARG:N	2.26	0.50
5:L:10:ILE:CD1	5:L:11:LEU:N	2.74	0.50
1:A:4:ARG:N	1:A:8:GLU:HB2	2.26	0.50
2:B:28:PRO:HD2	2:B:29:TRP:CE2	2.46	0.50
2:B:47:ILE:HG22	2:B:121:VAL:CG1	2.42	0.50
2:B:184(A):TYR:CE1	2:B:186(D):LYS:HB2	2.47	0.50
2:E:60:LEU:CA	2:E:60(F):LYS:O	2.60	0.50
2:E:215:TRP:HB2	6:E:1:0G6:C	2.42	0.50
4:K:87:LEU:HD22	4:K:90:GLU:CB	2.42	0.50
2:B:18:GLU:HB2	2:B:188:GLY:HA3	1.92	0.50
2:B:180:MET:HE2	2:B:215:TRP:NE1	2.26	0.50
2:E:145:LYS:CE	2:E:147:THR:HA	2.42	0.50
2:E:229:THR:HG22	2:E:230:HIS:N	2.27	0.50
3:J:50:ARG:HG2	3:J:50:ARG:NH1	2.25	0.50
2:B:58:CYS:SG	2:B:195:SER:HB2	2.51	0.49
4:H:78:THR:HG23	4:H:81:GLN:CG	2.41	0.49
5:I:11:LEU:HD22	5:L:2:VAL:C	2.36	0.49
4:K:95:ASN:O	4:K:99:GLU:HB2	2.12	0.49
2:B:31:VAL:CG1	2:B:66:VAL:HB	2.42	0.49
2:B:32:MET:CG	2:B:40:LEU:HD13	2.39	0.49
2:B:54:THR:OG1	2:B:55:ALA:N	2.44	0.49
2:B:127:GLU:O	2:B:128:THR:C	2.55	0.49
2:E:45:SER:CB	2:E:53:LEU:HB3	2.41	0.49
2:E:181:PHE:CD2	2:E:228:TYR:O	2.65	0.49
3:G:58:VAL:CG1	3:G:59:ASN:N	2.76	0.49
3:J:64:ASN:O	3:J:68:LYS:N	2.38	0.49
2:B:179:ASN:OD1	2:B:234:LEU:HD21	2.12	0.49
2:B:208:TYR:HB3	2:B:210:MET:SD	2.52	0.49
2:E:167:VAL:HG12	2:E:225:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:28:PHE:O	5:L:32:TYR:HB2	2.12	0.49
2:B:30:GLN:HG2	2:B:155:LEU:CD2	2.42	0.49
2:B:60:LEU:HD12	2:B:60(F):LYS:O	2.13	0.49
2:B:122:CYS:HB3	2:B:208:TYR:CE2	2.47	0.49
2:B:123:LEU:C	2:B:208:TYR:CE2	2.90	0.49
2:E:99:LEU:HG	6:E:1:OG6:CZ	2.42	0.49
2:E:142:GLY:O	2:E:143:ASN:O	2.30	0.49
2:E:231:VAL:O	2:E:232:PHE:C	2.55	0.49
2:B:76:TYR:HE2	2:B:77(A):ARG:HA	1.77	0.49
2:E:143:ASN:HD22	2:E:192:GLU:HB2	1.78	0.49
5:L:19:CYS:HB3	5:L:20:PRO:CD	2.43	0.49
2:B:132:ALA:C	2:B:134:TYR:H	2.20	0.49
2:E:16:ILE:N	2:E:194:ASP:OD2	2.46	0.49
2:E:56:ALA:HB2	2:E:103:ILE:H	1.77	0.49
2:E:87:LYS:HB3	2:E:89:TYR:CZ	2.47	0.49
2:E:145:LYS:HD3	2:E:149(B):ASN:HB3	1.93	0.49
5:I:14:ARG:HB3	5:L:28:PHE:HE1	1.77	0.49
3:J:52:LYS:CG	4:K:62:ALA:HB3	2.41	0.49
1:A:14(D):ARG:HH22	1:A:15:ARG:HG2	1.77	0.49
2:B:33:LEU:CD2	2:B:41:LEU:HD11	2.42	0.49
1:D:14(D):ARG:HB3	1:D:14(H):GLU:HG3	1.93	0.49
2:E:137:ARG:C	2:E:138:VAL:HG23	2.36	0.49
2:E:239:GLN:O	2:E:240:LYS:C	2.52	0.49
3:G:36:CYS:SG	4:K:66:LEU:C	2.96	0.49
2:B:51:TRP:CZ2	2:B:246:GLY:HA2	2.43	0.49
2:E:125:ASP:OD1	2:E:128:THR:N	2.46	0.49
3:G:58:VAL:HG13	3:G:62:PHE:CD1	2.47	0.49
1:A:14(C):GLU:OE2	2:B:202:LYS:HE2	2.13	0.49
2:B:33:LEU:HB3	2:B:41:LEU:HD11	1.95	0.49
2:E:34:PHE:HD1	2:E:40:LEU:HA	1.76	0.49
3:G:41:TRP:HA	3:G:41:TRP:CE3	2.46	0.49
4:K:57:ARG:NH1	4:K:59:ALA:HA	2.28	0.49
3:G:52:LYS:HA	3:G:55:ILE:HD12	1.95	0.49
3:G:63:THR:O	3:G:66:ILE:HB	2.12	0.49
4:H:103:ASN:O	4:H:103:ASN:ND2	2.46	0.49
2:B:138:VAL:CG1	2:B:198:PRO:O	2.56	0.48
2:E:60(B):PRO:O	2:E:60(E):ASP:N	2.39	0.48
2:E:68:ILE:N	2:E:81:LYS:O	2.46	0.48
2:E:90:ILE:HD11	2:E:94:TYR:HD2	1.76	0.48
3:J:46:PRO:CB	5:L:22:THR:HB	2.40	0.48
1:A:14(G):LEU:HD13	1:A:14(J):TYR:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:PRO:HG2	2:B:29:TRP:CE3	2.47	0.48
2:B:239:GLN:HE21	2:B:240:LYS:HE3	1.78	0.48
2:E:49:ASP:OD1	2:E:50:ARG:NE	2.46	0.48
2:E:177:THR:HB	2:E:180:MET:HB2	1.96	0.48
3:G:32:ASP:O	3:G:33:TRP:HE3	1.97	0.48
5:L:10:ILE:O	5:L:11:LEU:C	2.56	0.48
1:A:4:ARG:NH2	2:B:207:TRP:CZ2	2.82	0.48
2:B:56:ALA:HA	2:B:104:ALA:HB2	1.95	0.48
2:B:200:VAL:O	2:B:201:MET:HG3	2.13	0.48
2:B:202:LYS:HE3	2:B:205:ASN:HB2	1.96	0.48
2:B:213:VAL:HG22	2:B:228:TYR:CE2	2.48	0.48
2:B:216:GLY:N	6:B:1:OG6:NE	2.58	0.48
2:E:204(B):ASN:OD1	2:E:206:ARG:HG3	2.12	0.48
4:K:87:LEU:HD22	4:K:90:GLU:HB2	1.95	0.48
1:A:14(F):LEU:CD2	2:B:202:LYS:H	2.26	0.48
2:B:137:ARG:HA	2:B:159:ASN:HA	1.96	0.48
2:E:57:HIS:N	2:E:102:ASP:OD1	2.37	0.48
2:E:161:PRO:HG2	2:E:184:GLY:O	2.13	0.48
4:H:89:GLN:O	4:H:92:PRO:HG2	2.13	0.48
1:A:14:ASP:OD2	1:A:14(C):GLU:HB2	2.12	0.48
2:B:165:ARG:HB3	2:B:169:LYS:HD2	1.96	0.48
2:B:204(B):ASN:HD22	2:B:204(B):ASN:N	2.08	0.48
1:D:13:GLU:HA	1:D:14(C):GLU:OE1	2.14	0.48
2:E:91:HIS:O	2:E:94:TYR:HB3	2.14	0.48
2:E:171:SER:HB2	2:E:224:LYS:HE2	1.93	0.48
5:L:2:VAL:CG1	5:L:3:ALA:H	2.07	0.48
1:A:14(G):LEU:HG	1:A:15:ARG:HD3	1.96	0.48
2:B:44:ALA:HB1	2:B:52:VAL:HG11	1.94	0.48
2:B:78:ASN:N	2:B:78:ASN:ND2	2.57	0.48
2:B:96:TRP:H	2:B:96:TRP:CD1	2.32	0.48
2:B:122:CYS:SG	2:B:206:ARG:HD2	2.53	0.48
2:B:171:SER:O	2:B:224:LYS:NZ	2.46	0.48
2:B:177:THR:HB	2:B:180:MET:HB2	1.94	0.48
3:J:63:THR:O	3:J:64:ASN:C	2.56	0.48
2:B:46:LEU:HD13	2:B:120:PRO:CA	2.43	0.48
2:B:236:LYS:O	2:B:237:TRP:C	2.57	0.48
1:D:14:ASP:O	1:D:14(A):LYS:C	2.55	0.48
2:E:167:VAL:HG11	2:E:185:LYS:HE3	1.94	0.48
1:A:4:ARG:HB2	1:A:8:GLU:CD	2.39	0.48
2:E:27:SER:OG	2:E:29:TRP:CD1	2.63	0.48
5:L:3:ALA:O	5:L:4:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:37:ASP:O	5:L:41:GLN:N	2.46	0.48
5:L:40:LEU:C	5:L:44:GLU:OE1	2.57	0.48
2:B:163:VAL:HG13	2:B:164:GLU:OE1	2.14	0.48
2:B:165:ARG:HB2	2:B:166:PRO:HD3	1.95	0.48
2:E:159:ASN:OD1	2:E:159:ASN:O	2.31	0.48
3:G:41:TRP:CH2	5:I:23:CYS:HA	2.49	0.48
2:B:181:PHE:O	2:B:181:PHE:CD1	2.67	0.48
1:D:14:ASP:CB	2:E:23:GLU:OE1	2.62	0.48
2:E:82:ILE:O	3:G:38:ASP:OD1	2.32	0.48
2:E:90:ILE:HD13	2:E:91:HIS:C	2.39	0.48
2:E:164:GLU:CD	2:E:164:GLU:H	2.22	0.48
2:B:38:GLN:CD	2:B:38:GLN:N	2.71	0.47
2:B:127:GLU:C	2:B:129:ALA:N	2.72	0.47
2:B:164:GLU:OE1	2:B:167:VAL:HG21	2.14	0.47
2:B:180:MET:O	2:B:181:PHE:HB3	2.14	0.47
2:B:192:GLU:HG2	2:B:192:GLU:H	1.39	0.47
2:E:195:SER:C	2:E:197:GLY:H	2.22	0.47
4:H:66:LEU:C	3:J:36:CYS:SG	2.97	0.47
4:H:75:LEU:HD12	3:J:36:CYS:SG	2.54	0.47
1:D:14(H):GLU:CD	1:D:15:ARG:H	2.22	0.47
2:E:68:ILE:HG22	2:E:69:GLY:N	2.29	0.47
2:E:92:PRO:C	2:E:94:TYR:H	2.22	0.47
3:J:47:SER:O	3:J:48:GLY:C	2.57	0.47
2:B:33:LEU:CG	2:B:41:LEU:HD11	2.44	0.47
2:B:38:GLN:HB3	3:J:35:PHE:CD1	2.49	0.47
2:B:143:ASN:N	2:B:194:ASP:OD2	2.47	0.47
2:B:239:GLN:HB3	2:B:243:ASP:OD1	2.15	0.47
2:E:204:PRO:CG	2:E:204(A):PHE:N	2.77	0.47
3:G:63:THR:O	3:G:64:ASN:C	2.57	0.47
4:K:90:GLU:O	4:K:91:ARG:C	2.57	0.47
4:K:93:ILE:O	4:K:94:ARG:C	2.57	0.47
2:B:143:ASN:ND2	2:B:147:THR:CG2	2.76	0.47
2:E:70:LYS:HE3	2:E:70:LYS:HB3	1.80	0.47
2:B:40:LEU:HD11	2:B:42:CYS:O	2.15	0.47
1:D:4:ARG:NH2	1:D:8:GLU:OE2	2.46	0.47
2:E:99:LEU:HD12	6:E:1:OG6:CE2	2.43	0.47
2:E:203:SER:O	2:E:205:ASN:N	2.48	0.47
5:L:37:ASP:O	5:L:40:LEU:N	2.47	0.47
2:B:127:GLU:O	2:B:129(B):SER:CB	2.62	0.47
2:B:231:VAL:HG12	2:B:232:PHE:N	2.29	0.47
2:E:85:LEU:CA	2:E:109:LYS:H	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:231:VAL:HG22	2:E:232:PHE:N	2.30	0.47
4:H:78:THR:HG23	4:H:81:GLN:HB2	1.95	0.47
1:A:14(G):LEU:HD13	1:A:14(J):TYR:CE2	2.50	0.47
2:B:215:TRP:CE3	2:B:216:GLY:CA	2.97	0.47
6:B:1:0G6:HD2	6:B:1:0G6:C	2.44	0.47
1:D:1(A):ASP:O	1:D:1(A):ASP:OD2	2.32	0.47
1:D:1:CYS:N	2:E:206:ARG:HH12	2.13	0.47
2:E:60(A):TYR:C	2:E:60(C):PRO:HD2	2.39	0.47
2:E:60(F):LYS:HG3	2:E:60(H):PHE:HD2	1.77	0.47
2:E:67:ARG:NH2	2:E:80:GLU:OE1	2.45	0.47
2:E:68:ILE:HG22	2:E:118:ILE:HD12	1.96	0.47
2:E:99:LEU:HD22	2:E:102:ASP:CG	2.39	0.47
2:E:165:ARG:CZ	2:E:178:ASP:HA	2.45	0.47
3:G:50:ARG:O	3:G:51:MET:C	2.58	0.47
5:I:19:CYS:HB3	5:I:20:PRO:HD2	1.97	0.47
2:B:138:VAL:CG1	2:B:139:THR:N	2.73	0.47
2:B:159:ASN:OD1	2:B:159:ASN:N	2.47	0.47
4:H:79:GLY:C	5:I:20:PRO:HD2	2.40	0.47
2:B:91:HIS:N	2:B:237:TRP:CZ2	2.83	0.47
3:G:29:LYS:O	3:G:30:ASP:C	2.58	0.47
3:J:64:ASN:OD1	3:J:68:LYS:HE3	2.14	0.47
2:B:34:PHE:CD1	2:B:40:LEU:HA	2.50	0.47
2:E:114:PHE:HA	2:E:118:ILE:CB	2.42	0.47
3:G:50:ARG:HH11	3:G:50:ARG:HG2	1.80	0.47
4:H:56:GLU:O	4:H:57:ARG:CB	2.62	0.47
2:B:18:GLU:HG3	2:B:187:ARG:C	2.40	0.46
2:B:87:LYS:HD2	2:B:89:TYR:CE1	2.50	0.46
4:K:90:GLU:O	4:K:93:ILE:HB	2.16	0.46
4:K:90:GLU:C	4:K:92:PRO:HD2	2.40	0.46
2:B:137:ARG:CB	2:B:200:VAL:HG22	2.43	0.46
2:B:172:THR:HG21	2:B:176:ILE:CG2	2.46	0.46
3:J:69:LEU:HD12	5:L:43:LEU:CD2	2.37	0.46
2:B:182:CYS:HA	2:B:226:GLY:O	2.16	0.46
3:G:43:TYR:HA	4:K:78:THR:CG2	2.46	0.46
3:G:45:CYS:HB3	5:I:22:THR:HB	1.97	0.46
3:G:49:CYS:N	4:H:77:PRO:HD2	2.30	0.46
4:K:90:GLU:O	4:K:93:ILE:N	2.48	0.46
4:K:91:ARG:N	4:K:92:PRO:HD2	2.31	0.46
2:E:181:PHE:O	2:E:227:PHE:HA	2.15	0.46
5:I:7:ASN:C	5:I:10:ILE:HD11	2.40	0.46
5:I:12:ASP:OD1	5:I:15:PHE:HD1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:54:LEU:O	3:J:58:VAL:HG23	2.16	0.46
2:B:35:ARG:NE	2:B:36(A):SER:O	2.48	0.46
2:B:189:ASP:CG	2:B:190:ALA:N	2.72	0.46
1:D:4:ARG:HD3	2:E:26:MET:O	2.15	0.46
2:E:58:CYS:O	2:E:60(F):LYS:HE2	2.16	0.46
2:E:60(A):TYR:HD2	2:E:60(D):TRP:HB2	1.80	0.46
2:E:101:ARG:C	2:E:103:ILE:HG22	2.41	0.46
2:E:203:SER:O	2:E:205:ASN:CA	2.64	0.46
5:I:33:GLN:O	5:I:36:VAL:HB	2.16	0.46
3:J:58:VAL:HG13	3:J:62:PHE:CE1	2.50	0.46
4:K:77:PRO:HB2	4:K:82:LEU:CD2	2.45	0.46
2:B:77(A):ARG:HH21	4:H:72:LEU:HD11	1.78	0.46
2:B:94:TYR:CZ	2:B:96:TRP:HB3	2.51	0.46
2:B:128:THR:CG2	2:B:129(C):LEU:HD22	2.46	0.46
2:B:238:ILE:O	2:B:241:VAL:CG2	2.51	0.46
2:E:180:MET:O	2:E:181:PHE:HB3	2.14	0.46
2:E:193:GLY:HA2	6:E:1:OG6:O2	2.15	0.46
2:B:56:ALA:HA	2:B:104:ALA:CB	2.46	0.46
2:E:61:GLU:N	2:E:88:ILE:HD11	2.30	0.46
2:E:184(A):TYR:CE2	2:E:186(D):LYS:HE3	2.50	0.46
4:H:101:ASN:O	4:H:105:GLU:N	2.48	0.46
3:J:55:ILE:HG13	5:L:29:LEU:HD22	1.96	0.46
2:B:16:ILE:HD11	2:B:190:ALA:HA	1.97	0.46
2:B:215:TRP:HA	6:B:1:OG6:CD3	2.40	0.46
2:E:184(A):TYR:CG	2:E:186(D):LYS:O	2.68	0.46
3:J:46:PRO:HD2	5:L:22:THR:CB	2.46	0.46
3:J:51:MET:O	3:J:54:LEU:N	2.49	0.46
3:J:65:ARG:HA	3:J:68:LYS:HB2	1.98	0.46
2:B:70:LYS:HB2	2:B:141:TRP:CZ2	2.51	0.46
2:E:35:ARG:HB3	2:E:39:GLU:HB2	1.97	0.46
2:E:129(B):SER:HB3	2:E:129(C):LEU:CD1	2.46	0.46
2:E:181:PHE:CE2	2:E:228:TYR:HB2	2.50	0.46
4:H:66:LEU:HD23	4:H:67:HIS:N	2.30	0.46
5:I:27:ASP:O	5:I:31:THR:OG1	2.34	0.46
4:K:69:ASP:OD2	4:K:70:PRO:N	2.49	0.46
1:A:4:ARG:HA	1:A:5:PRO:HD3	1.86	0.46
2:B:191:CYS:CA	6:B:1:OG6:HH22	2.27	0.46
2:E:73:ARG:HD3	2:E:152:PRO:O	2.16	0.46
2:E:182:CYS:SG	2:E:225:TYR:CD2	3.09	0.46
4:H:86:LEU:HD11	5:I:25:ILE:CG2	2.38	0.46
3:J:62:PHE:O	3:J:66:ILE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:SER:O	2:B:47:ILE:HD13	2.16	0.45
2:B:57:HIS:CG	6:B:1:OG6:HB31	2.51	0.45
2:B:142:GLY:CA	2:B:194:ASP:OD2	2.56	0.45
2:E:47:ILE:CG2	2:E:121:VAL:HG12	2.47	0.45
5:L:19:CYS:HB3	5:L:20:PRO:HD2	1.97	0.45
2:B:50:ARG:HG2	2:B:108:LEU:H	1.80	0.45
2:E:57:HIS:HB3	2:E:102:ASP:CG	2.40	0.45
2:E:136:GLY:O	2:E:160:LEU:N	2.48	0.45
2:E:230:HIS:O	2:E:234:LEU:HB2	2.16	0.45
3:G:52:LYS:O	3:G:53:GLY:C	2.60	0.45
2:B:33:LEU:HB3	2:B:41:LEU:CD1	2.46	0.45
2:B:122:CYS:O	2:B:208:TYR:HD2	1.98	0.45
2:B:124:PRO:O	2:B:235:LYS:NZ	2.50	0.45
2:E:18:GLU:HB2	2:E:188:GLY:HA3	1.97	0.45
2:E:52:VAL:O	2:E:106:MET:SD	2.74	0.45
2:E:105:LEU:HD23	2:E:106:MET:H	1.81	0.45
2:E:160:LEU:HB2	2:E:161:PRO:HD2	1.98	0.45
2:E:173:ARG:HG3	2:E:173:ARG:O	2.16	0.45
2:E:191:CYS:SG	2:E:192:GLU:N	2.76	0.45
4:H:90:GLU:HB2	5:I:32:TYR:HE1	1.82	0.45
5:I:36:VAL:O	5:I:37:ASP:C	2.60	0.45
2:B:35:ARG:O	2:B:36:LYS:C	2.60	0.45
2:B:180:MET:HE2	2:B:215:TRP:CD1	2.52	0.45
2:B:189:ASP:HB3	2:B:221(A):ASP:HB2	1.99	0.45
2:E:29:TRP:CA	2:E:46:LEU:HB3	2.45	0.45
4:K:67:HIS:H	4:K:73:GLY:C	2.23	0.45
2:B:47:ILE:HD13	2:B:52:VAL:HA	1.99	0.45
2:E:25:GLY:O	2:E:26:MET:C	2.60	0.45
2:E:35:ARG:CZ	2:E:36(A):SER:O	2.65	0.45
2:E:57:HIS:CB	2:E:102:ASP:OD1	2.58	0.45
2:E:96:TRP:H	2:E:96:TRP:CD1	2.35	0.45
2:E:236:LYS:O	2:E:239:GLN:NE2	2.49	0.45
4:H:67:HIS:O	4:H:68:ALA:C	2.59	0.45
2:B:16:ILE:N	2:B:194:ASP:OD1	2.50	0.45
2:E:77(A):ARG:C	2:E:79:ILE:H	2.25	0.45
5:I:7:ASN:OD1	5:I:17:SER:HB2	2.17	0.45
5:I:31:THR:O	5:I:32:TYR:C	2.59	0.45
3:J:29:LYS:O	3:J:29:LYS:CG	2.64	0.45
3:J:61:ASP:C	3:J:65:ARG:HD3	2.42	0.45
2:B:33:LEU:CD2	2:B:41:LEU:HD21	2.46	0.45
2:B:46:LEU:CD2	2:B:46:LEU:C	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:MET:C	2:B:85:LEU:HD23	2.41	0.45
2:B:237:TRP:O	2:B:240:LYS:HB2	2.16	0.45
1:D:14:ASP:O	1:D:14(B):THR:N	2.50	0.45
3:G:61:ASP:HA	3:G:64:ASN:HD21	1.81	0.45
4:H:67:HIS:HB2	4:H:75:LEU:CG	2.46	0.45
3:J:64:ASN:HA	3:J:67:ASN:HD22	1.78	0.45
1:A:1(C):GLU:O	1:A:1(B):ALA:CB	2.63	0.45
2:B:177:THR:HG21	2:B:179:ASN:HB2	1.99	0.45
2:B:215:TRP:CG	6:B:1:OG6:HD2	2.51	0.45
2:B:215:TRP:HB3	6:B:1:OG6:HA1	1.99	0.45
5:L:2:VAL:HG22	5:L:3:ALA:N	2.32	0.45
2:B:32:MET:CE	2:B:40:LEU:HD22	2.46	0.45
2:B:62:ASN:N	2:B:62:ASN:HD22	2.05	0.45
2:B:91:HIS:HB2	2:B:237:TRP:CE2	2.52	0.45
2:B:128:THR:HG22	2:B:129(C):LEU:HD13	1.98	0.45
2:B:198:PRO:CA	2:B:209:GLN:HG3	2.47	0.45
1:D:1(C):GLU:C	1:D:1(A):ASP:H	2.24	0.45
1:D:7:PHE:HB3	1:D:8:GLU:OE2	2.17	0.45
2:E:60(C):PRO:CG	2:E:96:TRP:CE3	3.00	0.45
2:E:114:PHE:HA	2:E:118:ILE:CG2	2.47	0.45
4:K:69:ASP:OD2	4:K:70:PRO:CD	2.64	0.45
2:B:45:SER:N	2:B:53:LEU:O	2.43	0.45
2:B:140:GLY:C	2:B:142:GLY:H	2.23	0.45
2:B:186(A):ASP:OD1	2:B:186(A):ASP:N	2.49	0.45
2:E:161:PRO:CG	2:E:184:GLY:O	2.65	0.45
3:G:45:CYS:HB3	3:G:46:PRO:CD	2.46	0.45
2:B:165:ARG:O	2:B:166:PRO:C	2.60	0.44
2:E:132:ALA:C	2:E:134:TYR:H	2.25	0.44
4:H:96:SER:HA	4:H:99:GLU:HB3	1.99	0.44
5:I:36:VAL:C	5:I:40:LEU:HG	2.41	0.44
1:A:14:ASP:OD2	1:A:14(C):GLU:CB	2.66	0.44
2:B:47:ILE:CD1	2:B:52:VAL:HA	2.47	0.44
2:B:50:ARG:CG	2:B:108:LEU:HB2	2.47	0.44
2:B:166:PRO:O	2:B:167:VAL:C	2.59	0.44
2:B:195:SER:C	2:B:197:GLY:N	2.75	0.44
2:E:90:ILE:HD13	2:E:91:HIS:O	2.16	0.44
2:E:93:ARG:HB3	2:E:101:ARG:NE	2.32	0.44
2:E:144:LEU:HD21	2:E:152:PRO:HD3	1.99	0.44
4:H:101:ASN:HA	4:H:104:VAL:CG1	2.47	0.44
4:K:87:LEU:HD22	4:K:87:LEU:HA	1.66	0.44
2:B:60(A):TYR:CE1	2:B:60(C):PRO:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:LYS:HA	2:B:160:LEU:O	2.17	0.44
2:B:236:LYS:HG3	2:B:237:TRP:N	2.29	0.44
2:E:16:ILE:HD13	2:E:190:ALA:HA	1.98	0.44
5:I:7:ASN:HB3	5:I:10:ILE:HD11	1.99	0.44
5:I:21:THR:O	5:I:22:THR:C	2.59	0.44
3:J:33:TRP:CE3	3:J:33:TRP:CA	3.00	0.44
3:J:50:ARG:O	3:J:51:MET:C	2.59	0.44
1:A:1:CYS:C	2:B:122:CYS:SG	3.00	0.44
1:A:2:GLY:N	2:B:122:CYS:SG	2.91	0.44
2:B:34:PHE:HD1	2:B:40:LEU:HA	1.81	0.44
2:E:81:LYS:HD2	2:E:81:LYS:HA	1.78	0.44
4:H:86:LEU:HD23	4:H:86:LEU:N	2.32	0.44
4:K:78:THR:OG1	4:K:80:CYS:HB2	2.17	0.44
5:L:29:LEU:O	5:L:30:SER:C	2.61	0.44
1:A:14:ASP:O	1:A:14(B):THR:N	2.51	0.44
2:B:23:GLU:H	2:B:26:MET:HE1	1.83	0.44
2:E:57:HIS:CG	6:E:1:OG6:HB31	2.51	0.44
3:J:41:TRP:O	3:J:42:ASN:HB2	2.17	0.44
3:J:53:GLY:HA3	4:K:60:PRO:HB2	1.99	0.44
2:B:135:LYS:CA	2:B:161:PRO:HA	2.38	0.44
2:B:185:LYS:HD2	2:B:186(B):GLU:OE1	2.17	0.44
2:B:232:PHE:O	2:B:233:ARG:C	2.59	0.44
2:E:33:LEU:HD23	2:E:65:LEU:O	2.18	0.44
2:E:60(B):PRO:N	2:E:60(C):PRO:CD	2.81	0.44
2:E:97:ARG:HG3	2:E:97:ARG:HH11	1.82	0.44
3:G:33:TRP:CE3	3:G:33:TRP:CA	3.00	0.44
2:B:123:LEU:HG	2:B:235:LYS:NZ	2.33	0.44
2:B:163:VAL:HG12	2:B:164:GLU:O	2.17	0.44
2:B:184(A):TYR:CE2	2:B:186(D):LYS:HB2	2.53	0.44
1:D:14(F):LEU:O	1:D:14(J):TYR:CD1	2.71	0.44
2:E:33:LEU:C	2:E:41:LEU:HD12	2.42	0.44
2:E:105:LEU:CD2	2:E:106:MET:H	2.31	0.44
2:E:184(A):TYR:O	2:E:185:LYS:O	2.35	0.44
5:I:29:LEU:HD12	5:I:29:LEU:HA	1.74	0.44
2:B:64:LEU:HD12	2:B:64:LEU:N	2.30	0.44
2:B:128:THR:C	2:B:129(B):SER:HB3	2.42	0.44
2:B:237:TRP:HA	2:B:240:LYS:CG	2.46	0.44
1:D:1:CYS:SG	2:E:206:ARG:NH1	2.91	0.44
2:E:46:LEU:HD22	2:E:47:ILE:H	1.77	0.44
2:E:137:ARG:O	2:E:200:VAL:N	2.50	0.44
2:E:137:ARG:C	2:E:138:VAL:CG2	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:149(E):LYS:N	2:E:149(E):LYS:HD2	2.32	0.44
3:G:43:TYR:O	3:G:44:LYS:CG	2.57	0.44
1:A:1(C):GLU:C	1:A:1(A):ASP:N	2.76	0.44
2:B:17:VAL:HG22	2:B:191:CYS:HB2	1.99	0.44
2:B:77(A):ARG:O	2:B:79:ILE:HD13	2.18	0.44
2:B:146:GLU:CB	2:B:149(B):ASN:HD21	2.29	0.44
2:B:204(B):ASN:ND2	2:B:204(B):ASN:N	2.59	0.44
2:E:60:LEU:HB2	2:E:60(G):ASN:HA	2.00	0.44
2:E:100:ASP:O	2:E:101:ARG:HB2	2.18	0.44
1:A:14(J):TYR:HA	2:B:134:TYR:CE1	2.53	0.43
2:B:31:VAL:HG13	2:B:68:ILE:HG13	2.00	0.43
2:E:31:VAL:HB	2:E:44:ALA:CB	2.19	0.43
2:E:46:LEU:HA	2:E:52:VAL:CG2	2.37	0.43
2:E:160:LEU:C	2:E:160:LEU:HD12	2.43	0.43
2:E:205:ASN:ND2	2:E:205:ASN:O	2.50	0.43
2:E:212:ILE:O	2:E:213:VAL:C	2.61	0.43
4:K:67:HIS:O	4:K:68:ALA:C	2.61	0.43
2:B:129(C):LEU:HD11	2:B:204(A):PHE:CE2	2.47	0.43
2:E:38:GLN:CD	2:E:38:GLN:H	2.25	0.43
2:E:84:MET:O	2:E:85:LEU:HD23	2.18	0.43
2:E:93:ARG:O	2:E:101:ARG:NH1	2.51	0.43
4:H:96:SER:O	4:H:99:GLU:HB3	2.17	0.43
2:B:23:GLU:CA	2:B:26:MET:HE3	2.47	0.43
2:B:41:LEU:HD12	2:B:41:LEU:C	2.37	0.43
2:B:60(B):PRO:O	2:B:60(C):PRO:C	2.58	0.43
2:B:67:ARG:HE	2:B:70:LYS:HE2	1.83	0.43
2:E:200:VAL:O	2:E:201:MET:HG3	2.17	0.43
3:G:42:ASN:O	3:G:43:TYR:CD1	2.72	0.43
3:G:62:PHE:CZ	5:I:33:GLN:HG2	2.53	0.43
2:B:51:TRP:HA	2:B:106:MET:O	2.19	0.43
2:B:108:LEU:HD12	2:B:110:LYS:O	2.19	0.43
2:B:209:GLN:HE22	2:B:212:ILE:HG13	1.83	0.43
2:E:67:ARG:HE	2:E:70:LYS:HD2	1.83	0.43
2:E:121:VAL:HG22	2:E:122:CYS:N	2.33	0.43
2:E:215:TRP:CE3	2:E:216:GLY:N	2.86	0.43
2:E:215:TRP:CG	6:E:1:OG6:HD2	2.53	0.43
3:J:46:PRO:HD2	5:L:22:THR:OG1	2.19	0.43
4:K:57:ARG:HG3	4:K:57:ARG:NH1	2.30	0.43
2:B:101:ARG:C	2:B:103:ILE:HG22	2.44	0.43
2:B:213:VAL:O	2:B:213:VAL:HG12	2.18	0.43
2:E:18:GLU:OE1	2:E:187:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:60(C):PRO:CG	2:E:96:TRP:CZ3	3.00	0.43
2:E:179:ASN:C	2:E:230:HIS:HB2	2.38	0.43
3:G:52:LYS:CG	4:H:62:ALA:HB3	2.47	0.43
4:H:75:LEU:CD1	3:J:36:CYS:SG	3.07	0.43
2:B:22:ALA:CA	2:B:157:VAL:HG23	2.48	0.43
2:E:33:LEU:CD1	2:E:41:LEU:HD13	2.27	0.43
2:E:195:SER:HA	2:E:213:VAL:HB	2.00	0.43
2:E:242:ILE:CG1	2:E:243:ASP:N	2.81	0.43
5:I:40:LEU:O	5:I:43:LEU:N	2.49	0.43
1:A:6:LEU:CD1	2:B:25:GLY:HA3	2.47	0.43
2:B:86:GLU:HB2	2:B:109:LYS:N	2.33	0.43
2:B:144:LEU:HD23	2:B:152:PRO:HD3	1.96	0.43
2:B:215:TRP:HB2	6:B:1:OG6:C	2.49	0.43
1:D:14(J):TYR:O	1:D:14(L):ASP:N	2.51	0.43
2:E:141:TRP:O	2:E:142:GLY:C	2.62	0.43
3:J:61:ASP:O	3:J:65:ARG:HD3	2.17	0.43
2:B:33:LEU:HD13	2:B:41:LEU:CD1	2.41	0.43
2:B:100:ASP:O	2:B:101:ARG:CB	2.66	0.43
1:D:4:ARG:HB3	1:D:7:PHE:HD2	1.84	0.43
1:D:14(E):GLU:O	1:D:14(I):SER:N	2.51	0.43
2:E:88:ILE:HG22	2:E:89:TYR:N	2.32	0.43
2:E:142:GLY:N	2:E:194:ASP:OD1	2.52	0.43
3:G:50:ARG:NH2	4:H:61:ASP:OD2	2.52	0.43
4:H:65:CYS:C	3:J:36:CYS:SG	3.02	0.43
1:D:14:ASP:N	1:D:14(C):GLU:OE1	2.51	0.43
2:E:45:SER:C	2:E:52:VAL:HG13	2.43	0.43
2:E:68:ILE:CD1	2:E:81:LYS:O	2.67	0.43
5:I:37:ASP:HA	5:I:40:LEU:CG	2.49	0.43
2:B:95:ASN:O	2:B:95:ASN:CG	2.62	0.43
2:E:45:SER:O	2:E:52:VAL:HG22	2.19	0.43
2:E:60:LEU:CB	2:E:60(F):LYS:O	2.66	0.43
2:E:91:HIS:CE1	2:E:93:ARG:HB2	2.54	0.43
2:E:103:ILE:CG1	2:E:104:ALA:N	2.82	0.43
2:E:164:GLU:CG	2:E:167:VAL:HG23	2.48	0.43
2:B:18:GLU:CG	2:B:187:ARG:HB3	2.40	0.42
1:D:14:ASP:HB2	2:E:23:GLU:OE1	2.18	0.42
2:E:54:THR:HG22	2:E:104:ALA:O	2.19	0.42
2:E:129(B):SER:HB3	2:E:129(C):LEU:HD13	2.00	0.42
3:G:44:LYS:C	4:K:75:LEU:HB3	2.44	0.42
4:H:78:THR:N	4:H:81:GLN:HB2	2.34	0.42
2:E:56:ALA:HB2	2:E:103:ILE:C	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:103:ILE:HD13	2:E:237:TRP:CZ3	2.55	0.42
3:G:52:LYS:O	3:G:55:ILE:HB	2.18	0.42
2:B:124:PRO:HA	2:B:208:TYR:CZ	2.54	0.42
2:B:182:CYS:O	2:B:183:ALA:CB	2.67	0.42
2:B:221(A):ASP:O	2:B:221(A):ASP:CG	2.61	0.42
2:E:29:TRP:O	2:E:31:VAL:HG23	2.18	0.42
2:E:67:ARG:NE	2:E:80:GLU:OE1	2.51	0.42
1:A:5:PRO:HA	1:A:9:LYS:HB2	2.00	0.42
1:A:14:ASP:OD1	1:A:14(B):THR:C	2.62	0.42
2:B:29:TRP:CB	2:B:46:LEU:HB3	2.49	0.42
1:D:6:LEU:N	1:D:6:LEU:HD12	2.35	0.42
2:E:60:LEU:HA	2:E:60(F):LYS:CG	2.48	0.42
2:E:61:GLU:CD	2:E:61:GLU:H	2.27	0.42
2:E:130:LEU:N	2:E:131:GLN:HE22	2.17	0.42
2:E:174:ILE:O	2:E:175:ARG:C	2.63	0.42
2:B:20:SER:O	2:B:22:ALA:N	2.52	0.42
2:B:50:ARG:HG2	2:B:108:LEU:HB2	2.02	0.42
2:B:128:THR:HG23	2:B:129(C):LEU:CD1	2.49	0.42
2:B:233:ARG:HG2	2:B:233:ARG:HH11	1.84	0.42
2:B:239:GLN:HE21	2:B:239:GLN:HB2	1.51	0.42
2:E:47:ILE:HD11	2:E:53:LEU:H	1.85	0.42
2:E:68:ILE:HD13	2:E:81:LYS:O	2.19	0.42
2:E:136:GLY:O	2:E:159:ASN:HA	2.19	0.42
3:G:46:PRO:CD	5:I:22:THR:HB	2.45	0.42
5:I:9:CYS:O	5:I:10:ILE:C	2.63	0.42
4:K:57:ARG:HD2	4:K:58:LYS:N	2.33	0.42
5:L:5:ARG:O	5:L:8:CYS:O	2.38	0.42
2:B:198:PRO:C	2:B:209:GLN:HG3	2.45	0.42
3:G:50:ARG:CD	3:G:54:LEU:HD21	2.49	0.42
2:B:22:ALA:HB2	2:B:157:VAL:CG2	2.42	0.42
2:B:32:MET:HG2	2:B:40:LEU:CD1	2.44	0.42
2:B:42:CYS:HB3	2:B:43:GLY:H	1.75	0.42
2:B:128:THR:CA	2:B:129(C):LEU:HD13	2.50	0.42
2:B:184(A):TYR:CZ	2:B:186(D):LYS:HE2	2.55	0.42
2:E:57:HIS:HA	2:E:94:TYR:OH	2.20	0.42
2:E:70:LYS:HZ1	2:E:77:GLU:HG3	1.84	0.42
2:E:171:SER:HB2	2:E:223:GLY:O	2.20	0.42
2:E:235:LYS:HG2	2:E:239:GLN:OE1	2.18	0.42
3:J:64:ASN:O	3:J:68:LYS:HG3	2.19	0.42
2:B:55:ALA:HB3	2:B:58:CYS:SG	2.60	0.42
2:B:128:THR:CG2	2:B:129(C):LEU:CD1	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:PHE:N	2:B:209:GLN:HG3	2.34	0.42
2:B:232:PHE:C	2:B:235:LYS:H	2.27	0.42
1:D:1:CYS:O	1:D:3:LEU:N	2.53	0.42
2:E:31:VAL:CG2	2:E:46:LEU:HB2	2.47	0.42
2:E:103:ILE:CD1	2:E:237:TRP:CZ3	3.03	0.42
2:E:235:LYS:C	2:E:239:GLN:OE1	2.63	0.42
2:E:236:LYS:HA	2:E:239:GLN:HE22	1.84	0.42
3:G:36:CYS:SG	4:K:66:LEU:O	2.78	0.42
4:H:90:GLU:HA	5:I:32:TYR:OH	2.19	0.42
4:K:69:ASP:OD2	4:K:69:ASP:C	2.63	0.42
5:L:21:THR:O	5:L:24:GLY:N	2.53	0.42
1:A:14(J):TYR:O	1:A:14(L):ASP:N	2.51	0.42
2:B:138:VAL:O	2:B:158:VAL:HG12	2.19	0.42
2:E:53:LEU:HA	2:E:53:LEU:HD12	1.64	0.42
2:E:60(A):TYR:O	2:E:60(B):PRO:C	2.63	0.42
2:E:91:HIS:CD2	2:E:237:TRP:CD2	3.08	0.42
2:E:108:LEU:O	2:E:109:LYS:C	2.61	0.42
2:E:126:ARG:HA	2:E:232:PHE:CE1	2.54	0.42
2:B:28:PRO:C	2:B:119:HIS:O	2.62	0.42
2:B:60(I):THR:O	2:B:61:GLU:C	2.63	0.42
2:B:147:THR:CG2	2:B:192:GLU:HG3	2.50	0.42
2:E:47:ILE:HD11	2:E:53:LEU:N	2.34	0.42
2:E:90:ILE:HD11	2:E:94:TYR:CB	2.50	0.42
2:E:124:PRO:HG2	2:E:235:LYS:HD3	2.00	0.42
2:E:215:TRP:CE3	2:E:216:GLY:CA	3.03	0.42
5:L:25:ILE:O	5:L:28:PHE:N	2.52	0.42
2:B:86:GLU:OE1	2:B:86:GLU:CA	2.67	0.41
2:E:239:GLN:HE21	2:E:239:GLN:HB2	1.41	0.41
2:E:51:TRP:HZ2	2:E:246:GLY:H	1.68	0.41
2:E:103:ILE:C	2:E:103:ILE:HD13	2.45	0.41
4:H:97:VAL:HG12	4:H:98:ASP:N	2.35	0.41
2:B:57:HIS:NE2	6:B:1:0G6:HB31	2.35	0.41
2:B:199:PHE:HB2	2:B:211:GLY:O	2.21	0.41
2:E:45:SER:N	2:E:53:LEU:O	2.49	0.41
2:E:60(D):TRP:O	2:E:60(E):ASP:C	2.64	0.41
2:E:91:HIS:CD2	2:E:237:TRP:CG	3.08	0.41
2:E:105:LEU:HD12	2:E:238:ILE:HG23	2.01	0.41
2:E:134:TYR:C	2:E:161:PRO:HA	2.45	0.41
2:E:146:GLU:C	2:E:149(B):ASN:ND2	2.79	0.41
2:E:225:TYR:O	2:E:227:PHE:CE1	2.73	0.41
4:H:67:HIS:CE1	4:H:69:ASP:H	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:79:GLY:O	4:H:80:CYS:C	2.60	0.41
4:K:95:ASN:O	4:K:96:SER:C	2.63	0.41
2:B:85:LEU:HD23	2:B:85:LEU:N	2.35	0.41
2:E:28:PRO:HB2	2:E:119:HIS:N	2.35	0.41
2:E:49:ASP:C	2:E:50:ARG:HG3	2.45	0.41
2:E:60(B):PRO:O	2:E:60(C):PRO:C	2.62	0.41
2:E:203:SER:HB3	2:E:204(B):ASN:HD21	1.86	0.41
2:E:234:LEU:O	2:E:235:LYS:C	2.63	0.41
3:G:60:GLN:OE1	3:G:61:ASP:OD1	2.38	0.41
1:A:14(F):LEU:O	1:A:14(G):LEU:C	2.62	0.41
2:B:194:ASP:OD2	2:B:194:ASP:N	2.53	0.41
1:D:14(B):THR:O	1:D:14(B):THR:OG1	2.33	0.41
2:E:145:LYS:CA	2:E:146:GLU:OE2	2.69	0.41
5:I:12:ASP:O	5:I:13:GLU:C	2.64	0.41
3:J:37:SER:O	3:J:40:ASP:N	2.50	0.41
2:B:141:TRP:CD1	2:B:155:LEU:N	2.88	0.41
2:E:16:ILE:HG21	2:E:156:GLN:HB3	2.01	0.41
2:E:64:LEU:H	2:E:64:LEU:HD12	1.86	0.41
2:E:76:TYR:HE2	2:E:77(A):ARG:HG2	1.84	0.41
2:E:99:LEU:HD22	2:E:102:ASP:CB	2.51	0.41
2:E:115:SER:N	2:E:118:ILE:HB	2.31	0.41
1:A:5:PRO:O	1:A:10:LYS:HG3	2.21	0.41
2:B:56:ALA:HB2	2:B:103:ILE:O	2.19	0.41
2:B:143:ASN:HD22	2:B:192:GLU:HG3	1.86	0.41
2:B:230:HIS:O	2:B:231:VAL:C	2.63	0.41
2:E:47:ILE:HG22	2:E:121:VAL:HG12	2.03	0.41
2:E:144:LEU:O	2:E:145:LYS:CB	2.68	0.41
2:E:202:LYS:HE3	2:E:205:ASN:HB2	2.03	0.41
3:J:55:ILE:HG12	4:K:86:LEU:HD21	2.03	0.41
2:B:90:ILE:HD11	2:B:94:TYR:CD2	2.56	0.41
2:B:228:TYR:CD1	2:B:228:TYR:N	2.87	0.41
3:G:45:CYS:HB3	5:I:23:CYS:N	2.35	0.41
3:J:60:GLN:O	3:J:61:ASP:C	2.61	0.41
2:B:91:HIS:HB2	2:B:237:TRP:CZ2	2.55	0.41
2:B:244:GLN:HA	2:B:244:GLN:HE21	1.85	0.41
2:E:77(A):ARG:O	2:E:78:ASN:HB2	2.21	0.41
2:E:122:CYS:SG	2:E:206:ARG:HD2	2.61	0.41
2:E:146:GLU:OE2	2:E:220:CYS:HB2	2.21	0.41
3:G:50:ARG:HD3	4:H:60:PRO:O	2.21	0.41
4:K:57:ARG:NH1	4:K:57:ARG:CG	2.84	0.41
2:B:135:LYS:HZ1	2:B:184(A):TYR:HE2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:60(C):PRO:C	2:E:60(E):ASP:H	2.29	0.41
2:E:182:CYS:HB3	2:E:227:PHE:CD1	2.55	0.41
2:E:232:PHE:CA	2:E:235:LYS:HB2	2.51	0.41
5:I:40:LEU:O	5:I:41:GLN:C	2.64	0.41
4:K:80:CYS:O	4:K:81:GLN:C	2.64	0.41
2:B:51:TRP:NE1	2:B:242:ILE:HG22	2.34	0.40
2:B:125:ASP:O	2:B:129:ALA:HB2	2.21	0.40
2:B:128:THR:O	2:B:129:ALA:O	2.39	0.40
2:B:215:TRP:C	6:B:1:OG6:NE	2.67	0.40
2:E:32:MET:HG3	2:E:40:LEU:CD1	2.51	0.40
2:E:139:THR:HG22	2:E:157:VAL:HA	2.03	0.40
5:I:21:THR:C	5:I:23:CYS:N	2.77	0.40
4:K:67:HIS:CE1	4:K:69:ASP:CB	3.03	0.40
2:B:129:ALA:O	2:B:129(A):ALA:C	2.63	0.40
2:B:137:ARG:CA	2:B:200:VAL:HG22	2.51	0.40
2:B:173:ARG:HA	2:B:173:ARG:HD2	1.64	0.40
2:E:141:TRP:CE2	2:E:155:LEU:HD13	2.56	0.40
2:B:31:VAL:HG21	2:B:52:VAL:CG2	2.51	0.40
2:B:49:ASP:HB3	2:B:114:PHE:CE1	2.56	0.40
2:B:68:ILE:H	2:B:68:ILE:CD1	2.32	0.40
2:B:137:ARG:O	2:B:200:VAL:HG13	2.21	0.40
2:E:103:ILE:HB	2:E:229:THR:HG21	2.03	0.40
2:E:184(A):TYR:CE1	2:E:186(B):GLU:HB3	2.55	0.40
2:E:199:PHE:O	2:E:209:GLN:HA	2.21	0.40
3:G:45:CYS:O	3:G:46:PRO:O	2.39	0.40
5:L:41:GLN:HA	5:L:44:GLU:CD	2.42	0.40
2:B:202:LYS:NZ	2:B:205:ASN:O	2.46	0.40
4:H:69:ASP:HA	4:H:70:PRO:HD3	1.93	0.40
4:H:98:ASP:C	4:H:101:ASN:ND2	2.79	0.40
3:J:51:MET:SD	3:J:54:LEU:HD12	2.61	0.40
3:J:67:ASN:O	3:J:71:ASN:HB2	2.22	0.40
1:A:1(A):ASP:N	2:B:206:ARG:HH12	2.19	0.40
1:A:14(D):ARG:HH11	1:A:14(D):ARG:HB3	1.87	0.40
2:B:128:THR:CG2	2:B:129(C):LEU:CD2	3.00	0.40
2:B:145:LYS:HG3	2:B:146:GLU:N	2.36	0.40
2:E:49:ASP:O	2:E:50:ARG:HG3	2.21	0.40
2:E:77:GLU:O	2:E:80:GLU:N	2.39	0.40
3:G:66:ILE:HD12	3:G:66:ILE:HA	1.77	0.40
3:J:54:LEU:HD23	4:K:60:PRO:CG	2.51	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	30/36 (83%)	16 (53%)	7 (23%)	7 (23%)	0	0
1	D	30/36 (83%)	16 (53%)	6 (20%)	8 (27%)	0	0
2	B	256/259 (99%)	179 (70%)	57 (22%)	20 (8%)	1	7
2	E	256/259 (99%)	174 (68%)	55 (22%)	27 (10%)	0	4
3	G	46/57 (81%)	27 (59%)	14 (30%)	5 (11%)	0	3
3	J	46/57 (81%)	28 (61%)	13 (28%)	5 (11%)	0	3
4	H	50/91 (55%)	36 (72%)	7 (14%)	7 (14%)	0	2
4	K	50/91 (55%)	36 (72%)	11 (22%)	3 (6%)	1	12
5	I	38/45 (84%)	22 (58%)	10 (26%)	6 (16%)	0	2
5	L	42/45 (93%)	29 (69%)	5 (12%)	8 (19%)	0	1
All	All	844/976 (86%)	563 (67%)	185 (22%)	96 (11%)	0	3

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1(C)	GLU
1	A	2	GLY
2	B	60(E)	ASP
2	B	127	GLU
2	B	129	ALA
2	B	144	LEU
2	B	145	LYS
2	B	147	THR
2	B	183	ALA
2	B	213	VAL
2	B	231	VAL
1	D	1(C)	GLU
1	D	11	SER
2	E	21	ASP

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Mol	Chain	Res	Type
2	E	22	ALA
2	E	36	LYS
2	E	129	ALA
2	E	143	ASN
2	E	145	LYS
2	E	183	ALA
2	E	185	LYS
2	E	213	VAL
2	E	231	VAL
3	G	29	LYS
3	G	46	PRO
4	H	57	ARG
4	H	101	ASN
5	I	32	TYR
3	J	29	LYS
5	L	11	LEU
5	L	40	LEU
1	A	1	CYS
1	A	11	SER
1	A	14(A)	LYS
1	A	14(M)	GLY
2	B	21	ASP
2	B	98	ASN
2	B	128	THR
2	B	133	GLY
2	B	142	GLY
1	D	2	GLY
1	D	14(M)	GLY
2	E	30	GLN
2	E	60(E)	ASP
2	E	142	GLY
2	E	187	ARG
2	E	195	SER
2	E	198	PRO
4	H	93	ILE
4	H	100	LEU
5	I	12	ASP
3	J	48	GLY
3	J	58	VAL
4	K	63	GLY
5	L	5	ARG
5	L	20	PRO

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Mol	Chain	Res	Type
5	L	41	GLN
2	B	111	PRO
2	B	143	ASN
2	B	198	PRO
1	D	1	CYS
1	D	7	PHE
1	D	12	LEU
4	H	95	ASN
5	I	13	GLU
3	J	46	PRO
4	K	90	GLU
5	L	4	THR
5	L	31	THR
1	A	12	LEU
2	B	187	ARG
2	B	205	ASN
2	E	18	GLU
2	E	127	GLU
2	E	238	ILE
3	J	51	MET
4	K	57	ARG
2	B	132	ALA
1	D	14(A)	LYS
2	E	48	SER
2	E	111	PRO
2	E	132	ALA
2	E	144	LEU
2	E	149(C)	VAL
2	E	189	ASP
2	E	236	LYS
3	G	30	ASP
5	I	40	LEU
2	E	232	PHE
4	H	63	GLY
3	G	48	GLY
3	G	53	GLY
5	I	36	VAL
5	L	36	VAL
4	H	60	PRO
5	I	20	PRO

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	28/31 (90%)	26 (93%)	2 (7%)	13	38
1	D	28/31 (90%)	11 (39%)	17 (61%)	0	0
2	B	221/225 (98%)	159 (72%)	62 (28%)	0	2
2	E	221/225 (98%)	159 (72%)	62 (28%)	0	2
3	G	44/53 (83%)	31 (70%)	13 (30%)	0	2
3	J	44/53 (83%)	32 (73%)	12 (27%)	0	3
4	H	41/72 (57%)	28 (68%)	13 (32%)	0	2
4	K	41/72 (57%)	36 (88%)	5 (12%)	5	21
5	I	36/41 (88%)	22 (61%)	14 (39%)	0	0
5	L	39/41 (95%)	33 (85%)	6 (15%)	2	14
All	All	743/844 (88%)	537 (72%)	206 (28%)	0	3

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	9	LYS
2	B	16	ILE
2	B	17	VAL
2	B	20	SER
2	B	27	SER
2	B	31	VAL
2	B	32	MET
2	B	34	PHE
2	B	36(A)	SER
2	B	38	GLN
2	B	46	LEU
2	B	47	ILE
2	B	48	SER
2	B	52	VAL
2	B	53	LEU

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Mol	Chain	Res	Type
2	B	61	GLU
2	B	62	ASN
2	B	63	ASP
2	B	64	LEU
2	B	65	LEU
2	B	68	ILE
2	B	70	LYS
2	B	72	SER
2	B	73	ARG
2	B	74	THR
2	B	75	ARG
2	B	78	ASN
2	B	84	MET
2	B	85	LEU
2	B	86	GLU
2	B	87	LYS
2	B	90	ILE
2	B	95	ASN
2	B	103	ILE
2	B	105	LEU
2	B	106	MET
2	B	108	LEU
2	B	114	PHE
2	B	119	HIS
2	B	120	PRO
2	B	123	LEU
2	B	131	GLN
2	B	139	THR
2	B	144	LEU
2	B	154	VAL
2	B	159	ASN
2	B	167	VAL
2	B	171	SER
2	B	172	THR
2	B	176	ILE
2	B	178	ASP
2	B	180	MET
2	B	184(A)	TYR
2	B	185	LYS
2	B	192	GLU
2	B	198	PRO
2	B	200	VAL

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Mol	Chain	Res	Type
2	B	201	MET
2	B	214	SER
2	B	224	LYS
2	B	239	GLN
2	B	240	LYS
2	B	242	ILE
1	D	1(C)	GLU
1	D	1(A)	ASP
1	D	1	CYS
1	D	9	LYS
1	D	14	ASP
1	D	14(A)	LYS
1	D	14(B)	THR
1	D	14(C)	GLU
1	D	14(D)	ARG
1	D	14(E)	GLU
1	D	14(F)	LEU
1	D	14(G)	LEU
1	D	14(H)	GLU
1	D	14(I)	SER
1	D	14(J)	TYR
1	D	14(K)	ILE
1	D	14(L)	ASP
2	E	16	ILE
2	E	17	VAL
2	E	20	SER
2	E	21	ASP
2	E	26	MET
2	E	29	TRP
2	E	31	VAL
2	E	33	LEU
2	E	36(A)	SER
2	E	38	GLN
2	E	41	LEU
2	E	45	SER
2	E	46	LEU
2	E	47	ILE
2	E	57	HIS
2	E	59	LEU
2	E	60	LEU
2	E	60(A)	TYR
2	E	60(B)	PRO

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Mol	Chain	Res	Type
2	E	60(C)	PRO
2	E	60(D)	TRP
2	E	60(E)	ASP
2	E	60(F)	LYS
2	E	60(G)	ASN
2	E	60(H)	PHE
2	E	60(I)	THR
2	E	62	ASN
2	E	64	LEU
2	E	68	ILE
2	E	72	SER
2	E	73	ARG
2	E	74	THR
2	E	81	LYS
2	E	86	GLU
2	E	90	ILE
2	E	97	ARG
2	E	97(A)	GLU
2	E	103	ILE
2	E	105	LEU
2	E	106	MET
2	E	110	LYS
2	E	114	PHE
2	E	123	LEU
2	E	125	ASP
2	E	129(B)	SER
2	E	129(C)	LEU
2	E	144	LEU
2	E	146	GLU
2	E	157	VAL
2	E	169	LYS
2	E	178	ASP
2	E	180	MET
2	E	198	PRO
2	E	200	VAL
2	E	217	GLU
2	E	224	LYS
2	E	225	TYR
2	E	234	LEU
2	E	236	LYS
2	E	239	GLN
2	E	241	VAL

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Mol	Chain	Res	Type
2	E	243	ASP
3	G	26	SER
3	G	28	CYS
3	G	32	ASP
3	G	33	TRP
3	G	34	PRO
3	G	35	PHE
3	G	47	SER
3	G	52	LYS
3	G	54	LEU
3	G	58	VAL
3	G	66	ILE
3	G	68	LYS
3	G	69	LEU
4	H	55	VAL
4	H	56	GLU
4	H	57	ARG
4	H	61	ASP
4	H	74	VAL
4	H	78	THR
4	H	81	GLN
4	H	89	GLN
4	H	101	ASN
4	H	102	ASN
4	H	103	ASN
4	H	104	VAL
4	H	105	GLU
5	I	8	CYS
5	I	9	CYS
5	I	13	GLU
5	I	21	THR
5	I	22	THR
5	I	30	SER
5	I	31	THR
5	I	33	GLN
5	I	34	THR
5	I	38	LYS
5	I	39	ASP
5	I	40	LEU
5	I	41	GLN
5	I	45	ASP
3	J	26	SER

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Mol	Chain	Res	Type
3	J	28	CYS
3	J	33	TRP
3	J	35	PHE
3	J	47	SER
3	J	51	MET
3	J	57	GLU
3	J	62	PHE
3	J	66	ILE
3	J	69	LEU
3	J	71	ASN
3	J	72	SER
4	K	66	LEU
4	K	74	VAL
4	K	78	THR
4	K	87	LEU
4	K	103	ASN
5	L	5	ARG
5	L	7	ASN
5	L	22	THR
5	L	33	GLN
5	L	41	GLN
5	L	43	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	60(G)	ASN
2	B	62	ASN
2	B	78	ASN
2	B	131	GLN
2	B	143	ASN
2	B	149(B)	ASN
2	B	151	GLN
2	B	204(B)	ASN
2	B	230	HIS
2	B	239	GLN
2	B	244	GLN
2	E	62	ASN
2	E	131	GLN
2	E	149(B)	ASN
2	E	151	GLN
2	E	204(B)	ASN

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Mol	Chain	Res	Type
3	G	42	ASN
3	G	67	ASN
4	H	83	GLN
4	H	101	ASN
4	H	103	ASN
5	I	41	GLN
3	J	42	ASN
3	J	60	GLN
3	J	67	ASN
4	K	81	GLN
4	K	101	ASN
4	K	103	ASN
5	L	41	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
7	PO4	E	2	-	4,4,4	1.43	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PO4	B	248	-	4,4,4	1.43	0	6,6,6	0.43	0
6	OG6	E	1	2	30,31,32	1.57	2 (6%)	37,41,42	0.62	0
6	OG6	B	1	2	30,31,32	1.76	1 (3%)	37,41,42	1.34	3 (8%)

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
6	OG6	E	1	2	-	4/31/41/43	0/2/2/2
6	OG6	B	1	2	-	2/31/41/43	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1	OG6	O2-C2	-7.98	1.22	1.43
6	E	1	OG6	O2-C2	-7.81	1.22	1.43
6	E	1	OG6	C3-C2	2.70	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1	OG6	C2-CA2-N2	-4.56	102.62	110.90
6	B	1	OG6	CB2-CG2-CD3	2.95	120.57	112.07
6	B	1	OG6	CE2-CD2-CG	2.56	124.21	120.61

There are no chirality outliers.

All (6) torsion outliers are listed below:

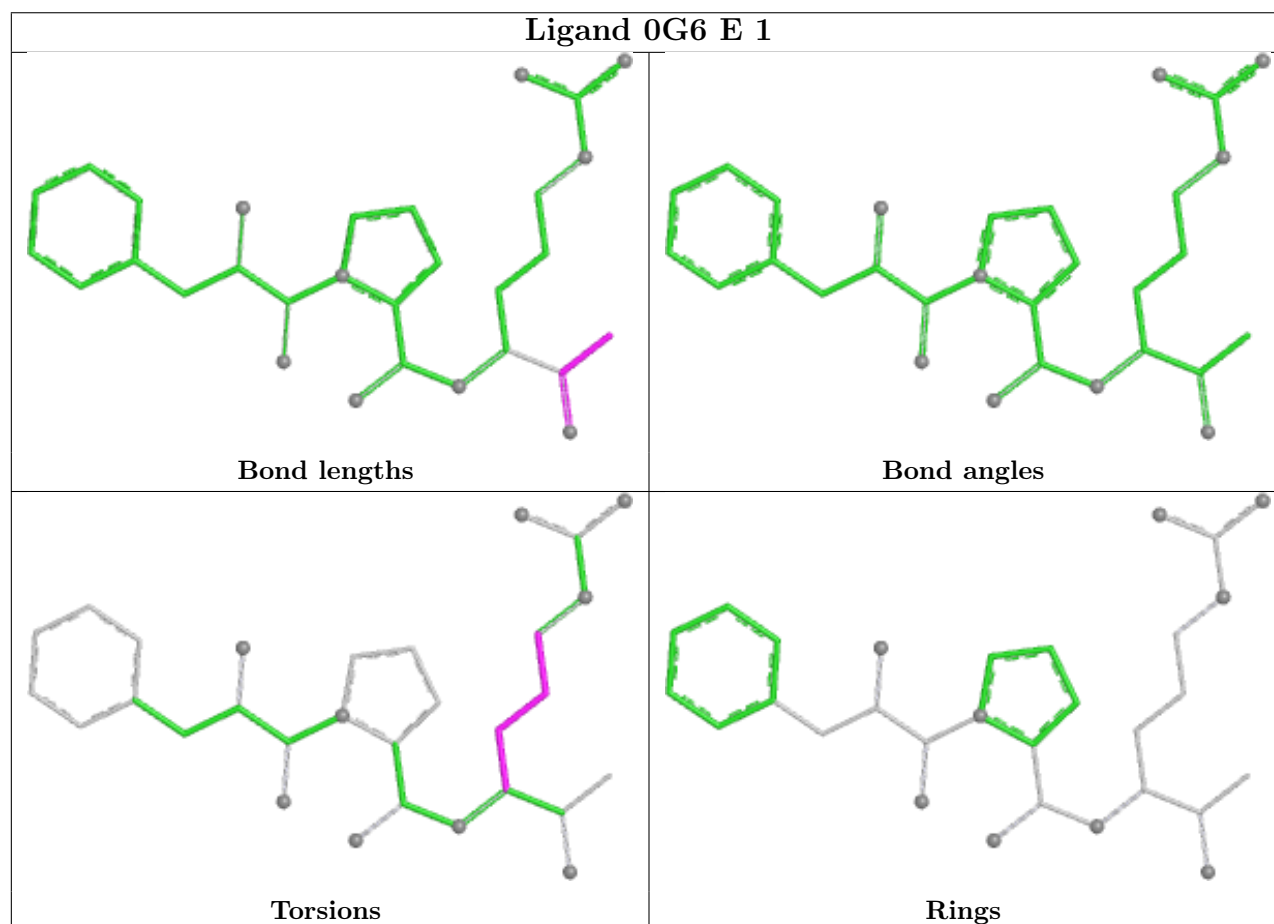
Mol	Chain	Res	Type	Atoms
6	B	1	OG6	CG2-CD3-NE-CZ1
6	B	1	OG6	NE-CD3-CG2-CB2
6	E	1	OG6	NE-CD3-CG2-CB2
6	E	1	OG6	C2-CA2-CB2-CG2
6	E	1	OG6	N2-CA2-CB2-CG2
6	E	1	OG6	CA2-CB2-CG2-CD3

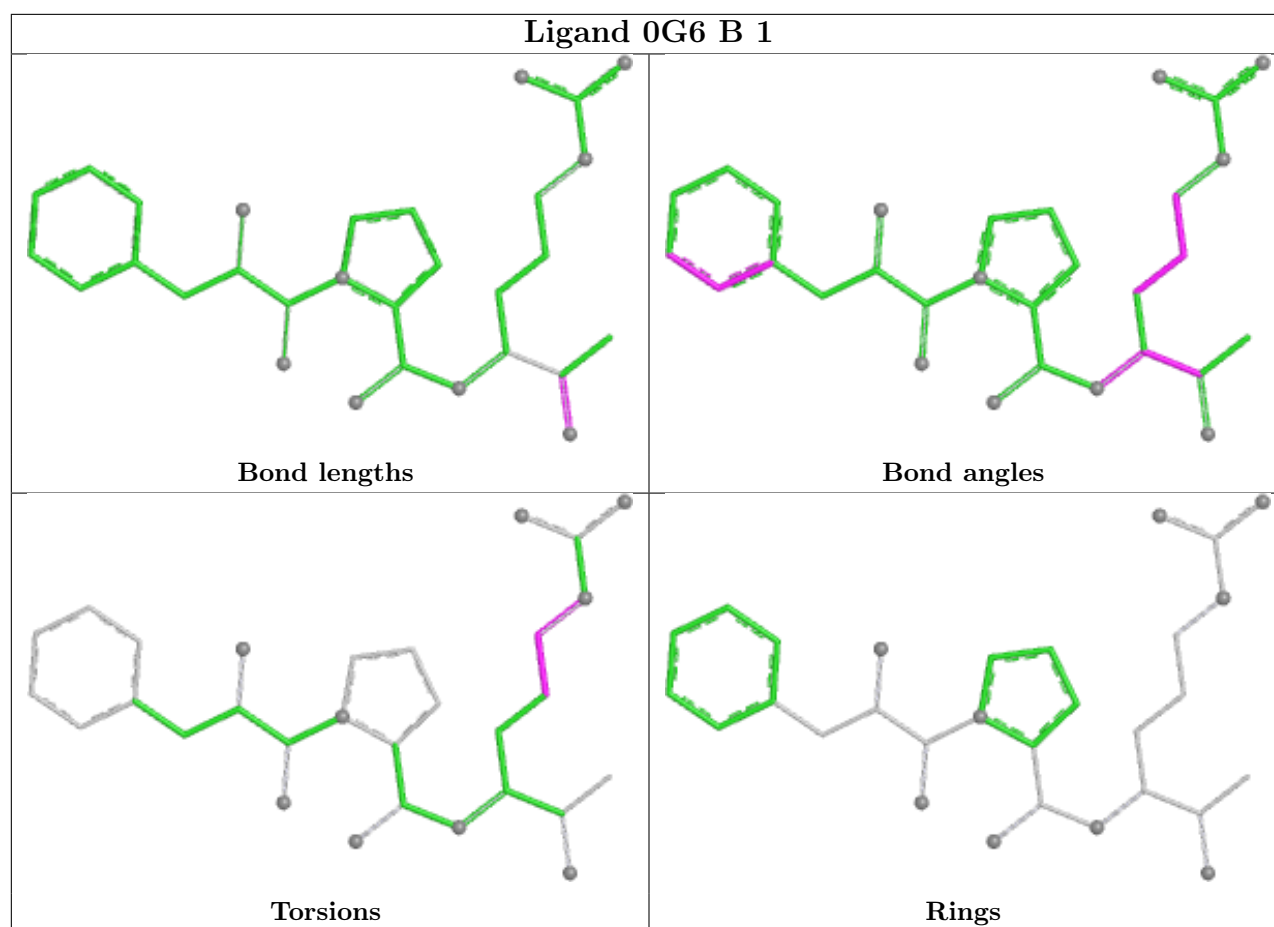
There are no ring outliers.

2 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1	0G6	19	0
6	B	1	0G6	33	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	32/36 (88%)	-1.29	0 100 100	28, 28, 28, 28	0
1	D	32/36 (88%)	-1.34	0 100 100	28, 28, 28, 28	0
2	B	258/259 (99%)	-1.31	0 100 100	28, 28, 28, 28	0
2	E	258/259 (99%)	-1.32	0 100 100	28, 28, 28, 28	0
3	G	45/57 (78%)	-1.38	0 100 100	28, 28, 28, 28	0
3	J	45/57 (78%)	-1.39	0 100 100	28, 28, 28, 28	0
4	H	52/91 (57%)	-1.35	0 100 100	28, 28, 28, 28	0
4	K	52/91 (57%)	-1.38	0 100 100	28, 28, 28, 28	0
5	I	40/45 (88%)	-1.35	0 100 100	28, 28, 28, 28	0
5	L	44/45 (97%)	-1.33	0 100 100	28, 28, 28, 28	0
All	All	858/976 (87%)	-1.33	0 100 100	28, 28, 28, 28	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

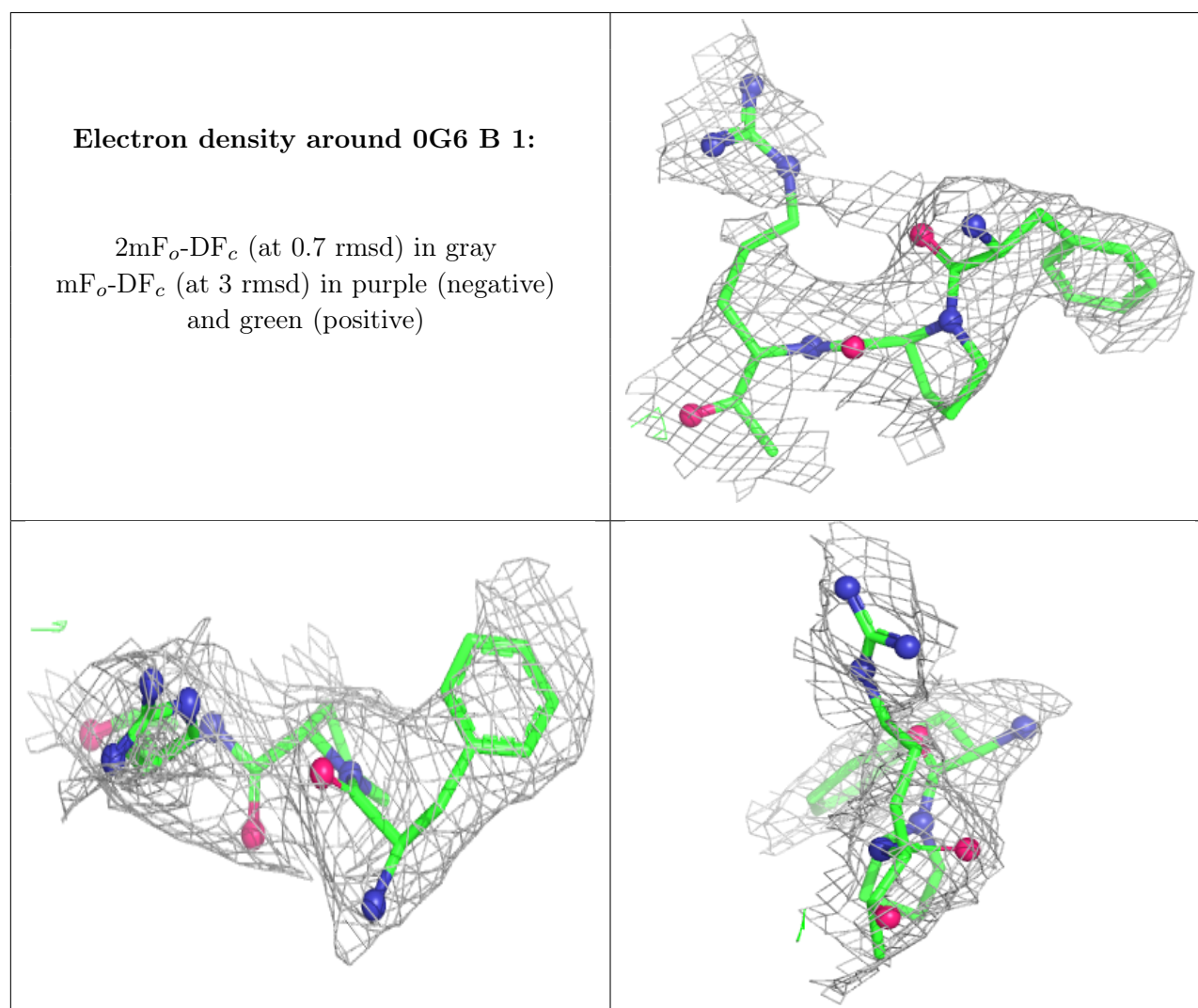
6.4 Ligands [i](#)

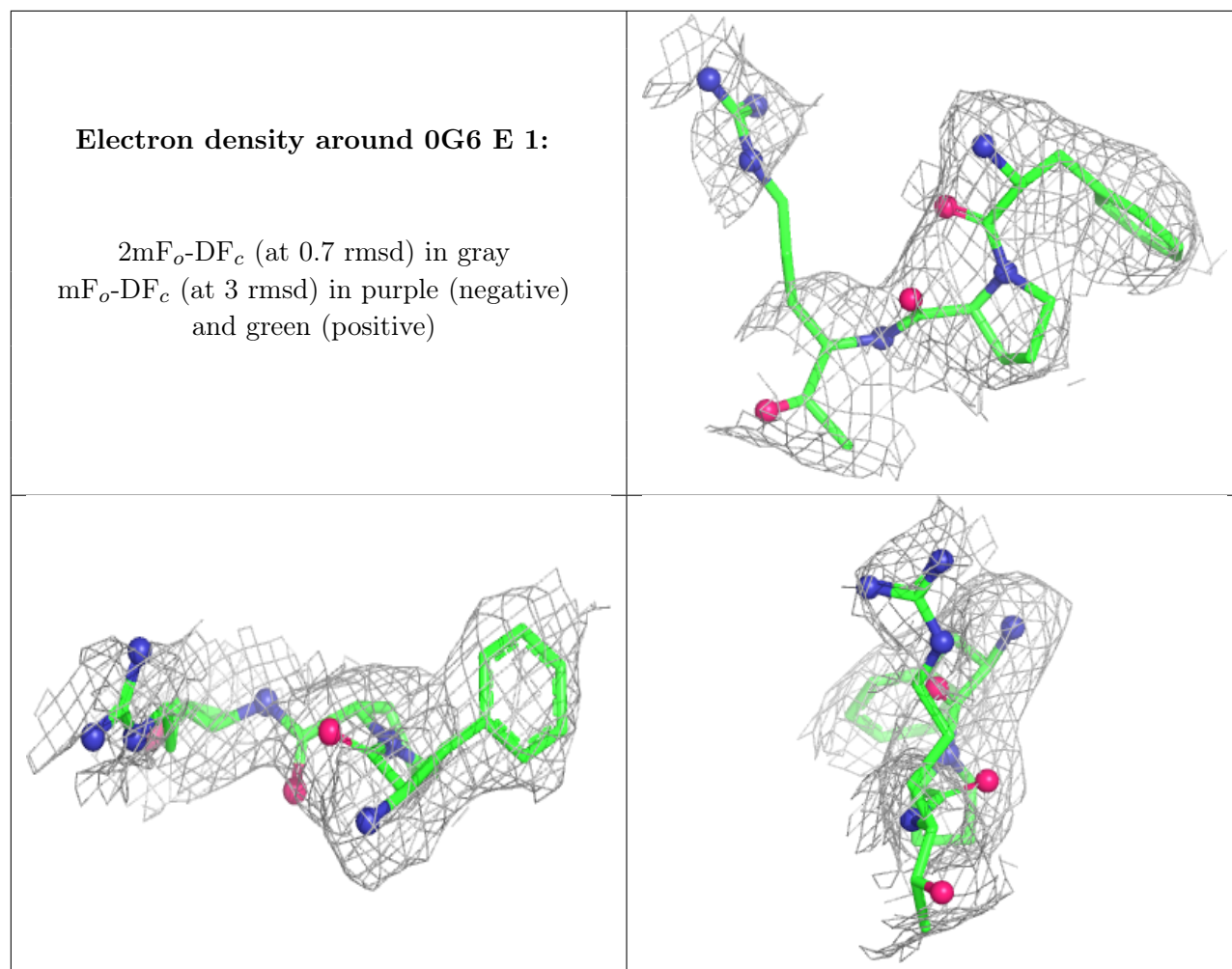
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
6	OG6	B	1	30/31	0.99	0.04	27,27,27,27	0
6	OG6	E	1	30/31	0.99	0.04	27,27,27,27	0
7	PO4	B	248	5/5	0.99	0.08	27,27,27,27	0
7	PO4	E	2	5/5	0.99	0.06	27,27,27,27	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.