



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:38 PM UTC

PDB ID : 4F52 / pdb_00004f52
Title : Structure of a Glomulin-RBX1-CUL1 complex
Authors : Duda, D.M.; Olszewski, J.L.; Schulman, B.A.
Deposited on : 2012-05-11
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

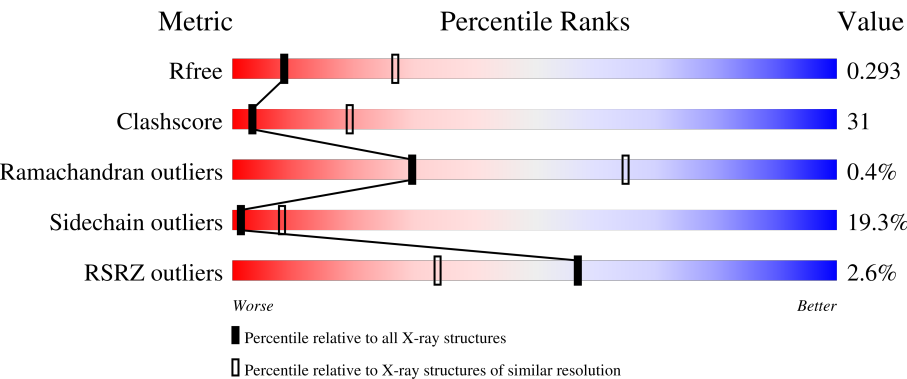
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	282	2% 44% 37% 10% 9%
1	C	282	4% 44% 38% 8% 10%
2	B	106	% 28% 44% 6% 21%
2	D	106	% 35% 35% 9% 20%
3	E	596	2% 37% 41% 9% 12%

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Mol	Chain	Length	Quality of chain
3	F	596	3% 32% 41% 12% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13897 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 Cullin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2103	1341	351	400	11			
1	C	254	Total	C	N	O	S	0	0	0
			2073	1326	345	392	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	GLY	-	expression tag	UNP Q13616
A	410	SER	-	expression tag	UNP Q13616
A	421	GLU	LEU	engineered mutation	UNP Q13616
A	451	GLU	VAL	engineered mutation	UNP Q13616
A	452	LYS	VAL	engineered mutation	UNP Q13616
A	455	LYS	TYR	engineered mutation	UNP Q13616
C	409	GLY	-	expression tag	UNP Q13616
C	410	SER	-	expression tag	UNP Q13616
C	421	GLU	LEU	engineered mutation	UNP Q13616
C	451	GLU	VAL	engineered mutation	UNP Q13616
C	452	LYS	VAL	engineered mutation	UNP Q13616
C	455	LYS	TYR	engineered mutation	UNP Q13616

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	84	Total	C	N	O	S	0	0	0
			692	438	127	118	9			
2	D	85	Total	C	N	O	S	0	0	0
			701	443	128	121	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	GLY	-	expression tag	UNP P62877
B	4	SER	-	expression tag	UNP P62877
D	3	GLY	-	expression tag	UNP P62877
D	4	SER	-	expression tag	UNP P62877

- Molecule 3 is a protein called Glomulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	523	Total	C	N	O	S	0	0	0
			4202	2720	685	772	25			
3	F	512	Total	C	N	O	S	0	0	0
			4120	2676	666	753	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP Q92990
E	0	SER	-	expression tag	UNP Q92990
F	-1	GLY	-	expression tag	UNP Q92990
F	0	SER	-	expression tag	UNP Q92990

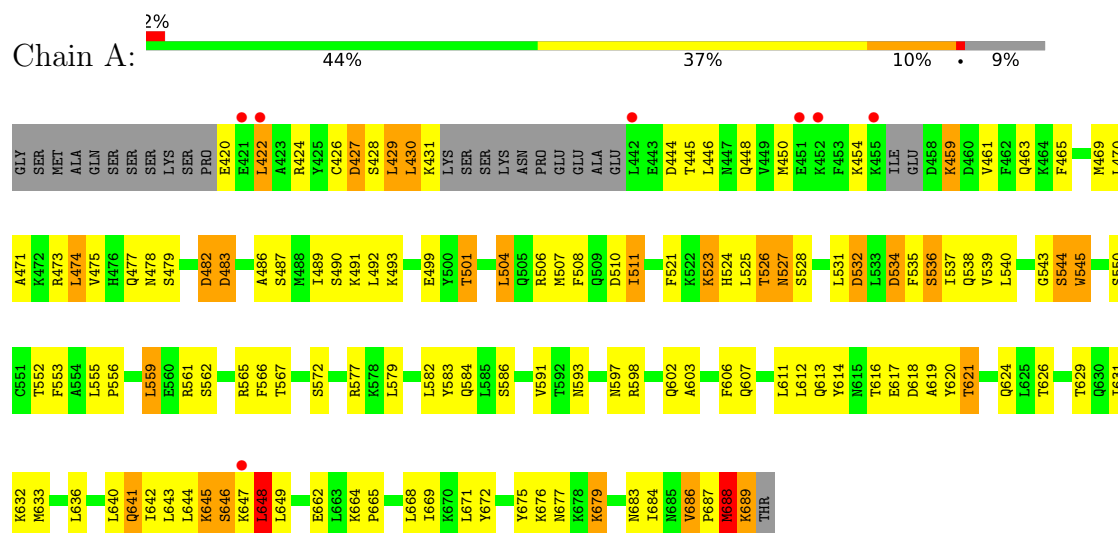
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Zn	0	0
			3	3		
4	D	3	Total	Zn	0	0
			3	3		

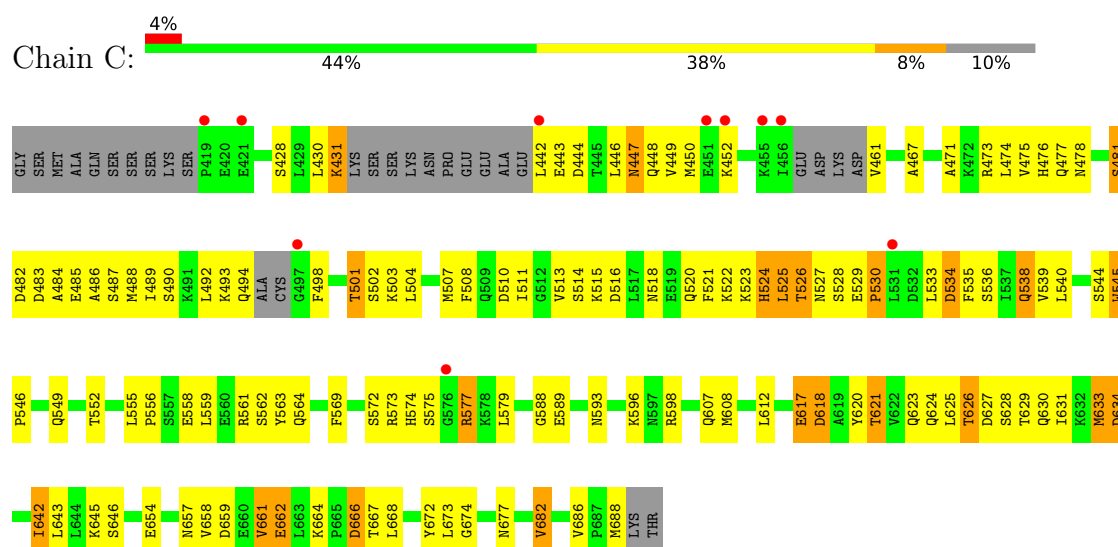
3 Residue-property plots

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: Cullin-1

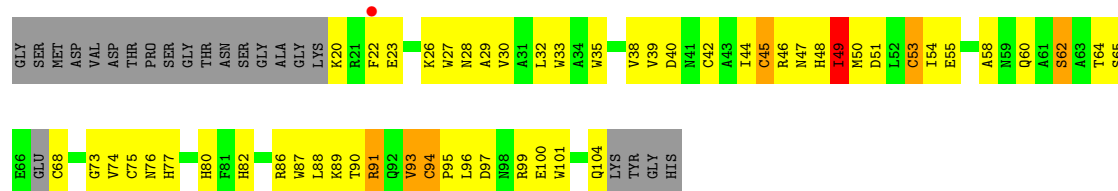


• Molecule 1: Cullin-1

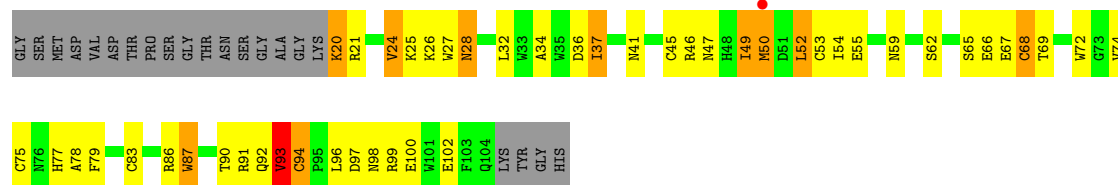


• Molecule 2: E3 ubiquitin-protein ligase RBX1

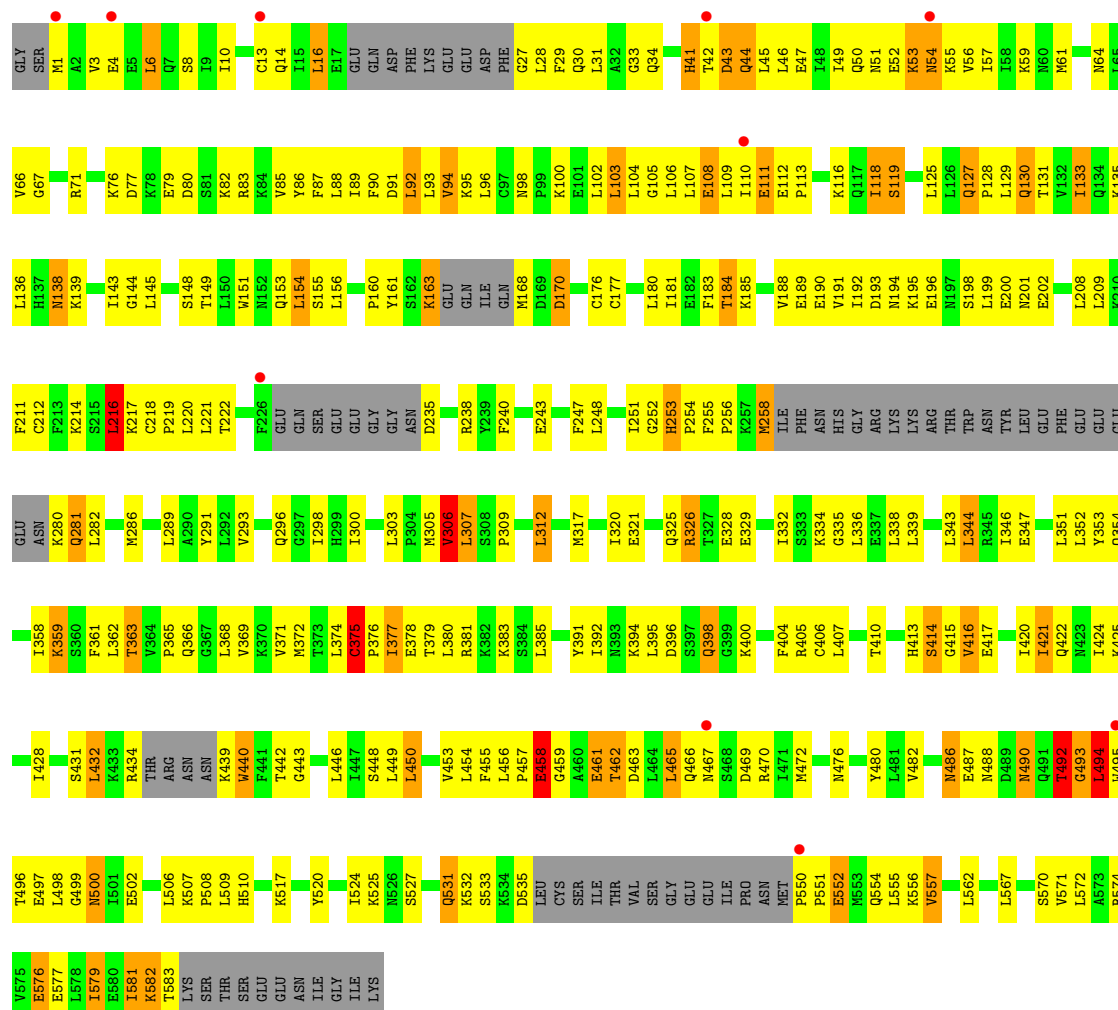




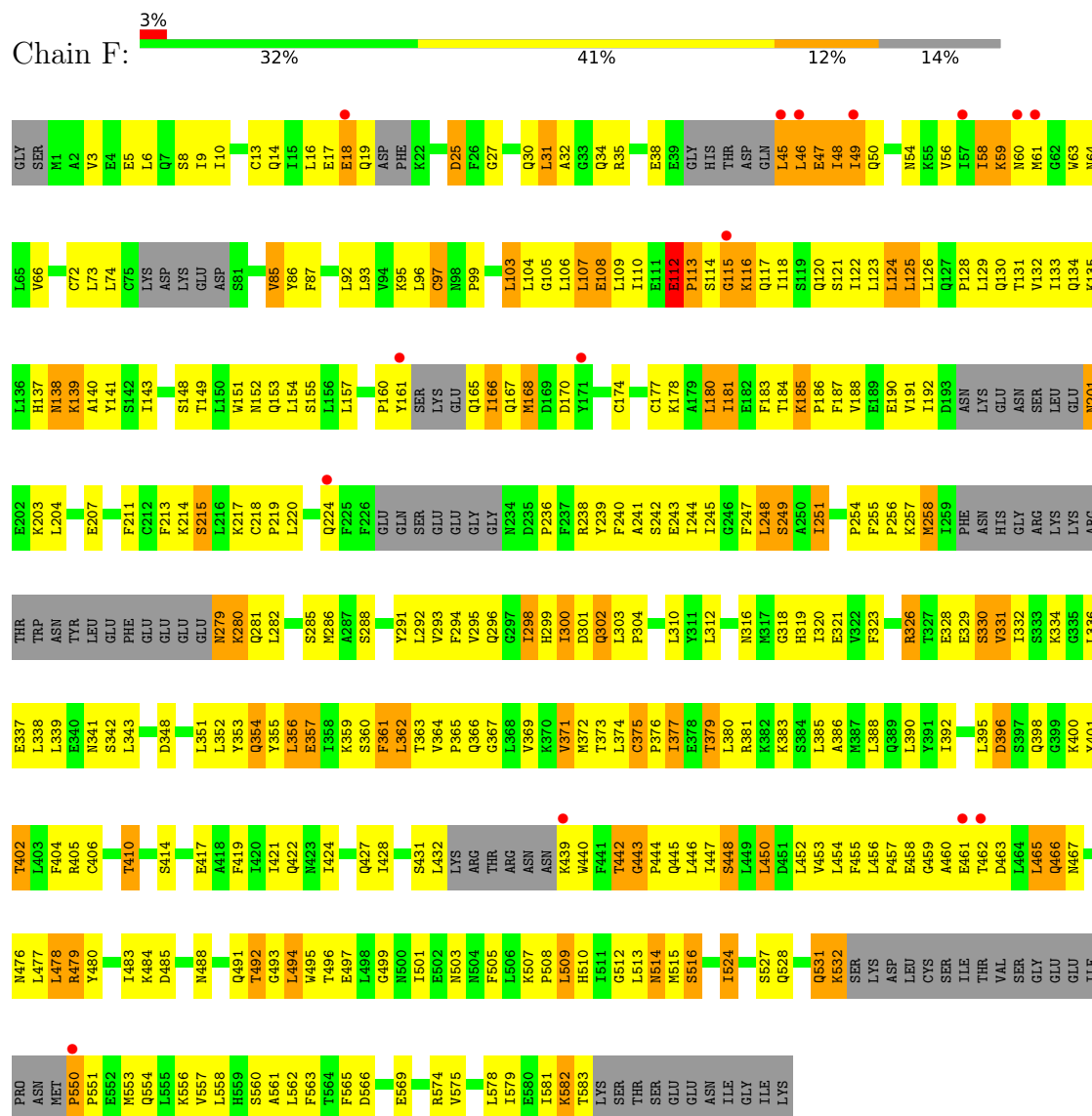
• Molecule 2: E3 ubiquitin-protein ligase RBX1



• Molecule 3: Glomulin



● Molecule 3: Glomulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.33Å 193.93Å 142.07Å 90.00° 98.81° 90.00°	Depositor
Resolution (Å)	37.39 – 3.00 37.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.39-3.00) 98.8 (37.39-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.219 , 0.289 0.230 , 0.293	Depositor DCC
R_{free} test set	2838 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	83.5	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 91.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13897	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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:
ZN

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	0.61	0/2136	0.98	10/2870 (0.3%)
1	C	0.53	0/2106	0.97	3/2830 (0.1%)
2	B	0.62	0/711	1.17	9/965 (0.9%)
2	D	0.58	0/721	1.06	4/980 (0.4%)
3	E	0.54	0/4269	1.02	15/5753 (0.3%)
3	F	0.50	0/4184	0.97	14/5639 (0.2%)
All	All	0.54	0/14127	1.00	55/19037 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	E	0	4
3	F	0	4
All	All	0	9

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	375	CYS	CA-C-N	11.47	132.40	119.32
3	E	375	CYS	C-N-CA	11.47	132.40	119.32
3	E	493	GLY	CA-C-N	8.94	132.26	120.28
3	E	493	GLY	C-N-CA	8.94	132.26	120.28
3	E	494	LEU	N-CA-C	8.21	120.23	111.28
3	F	375	CYS	CA-C-N	7.63	127.52	119.05
3	F	375	CYS	C-N-CA	7.63	127.52	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	ASN	N-CA-C	7.51	122.62	113.38
1	C	545	TRP	CA-C-N	7.46	127.17	119.56
1	C	545	TRP	C-N-CA	7.46	127.17	119.56
2	B	94	CYS	CA-C-N	7.36	127.00	119.19
2	B	94	CYS	C-N-CA	7.36	127.00	119.19
2	D	94	CYS	CA-C-N	7.10	126.36	118.97
2	D	94	CYS	C-N-CA	7.10	126.36	118.97
2	B	97	ASP	N-CA-C	-6.71	99.46	109.86
3	E	16	LEU	N-CA-C	6.29	119.03	110.35
3	F	288	SER	N-CA-C	-6.15	104.49	111.07
3	E	138	ASN	N-CA-C	6.13	117.97	111.28
2	B	97	ASP	CA-C-N	-5.98	114.34	123.07
2	B	97	ASP	C-N-CA	-5.98	114.34	123.07
2	B	100	GLU	N-CA-C	-5.92	102.30	110.35
1	A	644	LEU	N-CA-C	-5.81	105.03	111.36
3	F	443	GLY	CA-C-N	5.78	126.17	119.47
3	F	443	GLY	C-N-CA	5.78	126.17	119.47
3	E	98	ASN	CA-C-N	5.76	125.44	119.05
3	E	98	ASN	C-N-CA	5.76	125.44	119.05
2	D	21	ARG	N-CA-C	5.75	118.28	111.33
3	F	374	LEU	N-CA-C	5.67	118.66	111.69
3	E	374	LEU	N-CA-C	5.63	120.31	113.38
1	C	575	SER	N-CA-C	5.51	117.75	111.02
1	A	645	LYS	N-CA-C	-5.50	105.28	111.28
3	F	361	PHE	N-CA-C	5.47	117.24	111.28
3	E	28	LEU	N-CA-C	-5.43	105.52	111.82
1	A	688	MET	N-CA-C	5.42	119.00	112.38
3	F	138	ASN	N-CA-C	5.38	117.22	111.36
1	A	648	LEU	N-CA-C	5.36	117.12	111.28
3	E	216	LEU	N-CA-C	-5.35	105.45	111.28
2	B	49	ILE	N-CA-C	-5.33	102.10	110.09
1	A	545	TRP	CA-C-N	5.31	125.63	119.47
1	A	545	TRP	C-N-CA	5.31	125.63	119.47
1	A	550	SER	CB-CA-C	-5.30	109.49	115.79
3	E	431	SER	CA-C-N	-5.26	115.35	123.14
3	E	431	SER	C-N-CA	-5.26	115.35	123.14
1	A	543	GLY	N-CA-C	5.22	118.95	112.64
3	E	458	GLU	N-CA-C	-5.22	104.19	111.39
3	F	168	MET	N-CA-C	5.21	117.64	111.33
2	B	45	CYS	N-CA-C	-5.20	102.30	110.36
3	F	550	PRO	CA-C-N	5.16	124.78	119.05
3	F	550	PRO	C-N-CA	5.16	124.78	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	371	VAL	CB-CA-C	-5.14	105.30	111.88
3	F	298	ILE	N-CA-C	5.14	115.37	108.17
3	F	258	MET	N-CA-C	-5.13	106.80	113.16
1	A	603	ALA	N-CA-C	5.09	116.93	109.24
2	D	93	VAL	N-CA-C	5.06	114.99	108.82
2	B	47	ASN	N-CA-C	-5.00	100.86	108.76

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	501	THR	Peptide
3	E	111	GLU	Peptide
3	E	432	LEU	Peptide
3	E	492	THR	Peptide
3	E	493	GLY	Peptide
3	F	112	GLU	Peptide
3	F	114	SER	Peptide
3	F	115	GLY	Peptide
3	F	492	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2103	0	2127	124	0
1	C	2073	0	2101	125	0
2	B	692	0	647	49	0
2	D	701	0	654	44	0
3	E	4202	0	4360	287	0
3	F	4120	0	4271	285	0
4	B	3	0	0	0	0
4	D	3	0	0	0	0
All	All	13897	0	14160	858	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 31.

All (858) 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:C:525:LEU:O	1:C:529:GLU:HB2	1.21	1.37
1:C:530:PRO:O	1:C:561:ARG:NH2	1.68	1.26
1:A:646:SER:OG	1:A:648:LEU:HD12	1.35	1.21
1:A:647:LYS:HB2	1:A:675:TYR:CE1	1.76	1.20
1:C:527:ASN:HD22	3:F:551:PRO:HB3	1.09	1.10
3:E:254:PRO:C	3:E:256:PRO:HD2	1.74	1.10
3:E:51:ASN:HB3	3:E:53:LYS:HD3	1.35	1.06
3:F:46:LEU:CD2	3:F:85:VAL:HG23	1.90	1.00
3:E:406:CYS:O	3:E:410:THR:HG22	1.62	0.98
3:E:494:LEU:HD12	3:E:495:TRP:N	1.76	0.98
1:C:527:ASN:HD22	3:F:551:PRO:CB	1.76	0.97
1:C:523:LYS:O	1:C:526:THR:HG23	1.64	0.95
3:E:372:MET:O	3:E:381:ARG:HD2	1.64	0.95
1:A:647:LYS:HB2	1:A:675:TYR:CD1	2.02	0.94
1:C:525:LEU:O	1:C:529:GLU:CB	2.15	0.94
3:F:460:ALA:HB1	3:F:515:MET:HE2	1.50	0.94
1:A:647:LYS:HB2	1:A:675:TYR:HE1	1.30	0.93
3:E:136:LEU:HD21	3:E:139:LYS:HG3	1.52	0.92
3:E:490:ASN:OD1	3:E:495:TRP:CD1	2.23	0.92
3:F:456:LEU:HD13	3:F:459:GLY:HA2	1.49	0.91
3:E:463:ASP:O	3:E:467:ASN:HB2	1.71	0.90
3:F:18:GLU:O	3:F:18:GLU:HG2	1.71	0.90
3:E:494:LEU:CD1	3:E:495:TRP:N	2.35	0.89
3:E:255:PHE:N	3:E:256:PRO:HD2	1.88	0.89
3:F:279:ASN:C	3:F:279:ASN:ND2	2.30	0.88
2:D:67:GLU:HG3	2:D:68:CYS:H	1.37	0.87
3:E:255:PHE:CE1	3:E:303:LEU:CD1	2.57	0.87
3:E:52:GLU:O	3:E:55:LYS:HD3	1.74	0.87
1:C:523:LYS:HA	1:C:526:THR:CG2	2.05	0.86
1:C:527:ASN:ND2	3:F:551:PRO:HB3	1.90	0.86
3:F:46:LEU:HD22	3:F:85:VAL:HG23	1.56	0.86
3:F:279:ASN:C	3:F:279:ASN:HD22	1.83	0.86
3:E:494:LEU:HD12	3:E:495:TRP:H	1.39	0.86
1:A:487:SER:OG	1:A:491:LYS:NZ	2.08	0.86
1:C:524:HIS:HD2	1:C:569:PHE:HD1	1.24	0.86
3:F:213:PHE:CE2	3:F:282:LEU:HD11	2.11	0.85
1:C:530:PRO:O	1:C:561:ARG:CZ	2.24	0.85
1:C:607:GLN:HG2	1:C:643:LEU:HD21	1.56	0.85
1:A:619:ALA:HB1	1:A:668:LEU:HD11	1.59	0.84
3:F:405:ARG:NH2	3:F:448:SER:OG	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:490:ASN:OD1	3:E:495:TRP:HD1	1.57	0.84
3:E:255:PHE:CE1	3:E:303:LEU:HD11	2.14	0.83
1:A:626:THR:HG22	1:A:636:LEU:HD23	1.59	0.83
3:E:108:GLU:OE1	3:E:109:LEU:N	2.12	0.83
3:F:329:GLU:HG3	3:F:380:LEU:HD11	1.62	0.81
3:F:476:ASN:OD1	3:F:479:ARG:NH1	2.13	0.81
3:E:359:LYS:O	3:E:363:THR:HG23	1.80	0.81
3:F:46:LEU:HD21	3:F:85:VAL:HG23	1.62	0.81
1:A:626:THR:HG22	1:A:636:LEU:CD2	2.11	0.81
3:E:154:LEU:HD11	3:E:176:CYS:HB3	1.63	0.80
3:E:362:LEU:O	3:E:365:PRO:HD2	1.82	0.80
3:F:369:VAL:HA	3:F:372:MET:HG2	1.63	0.80
3:F:494:LEU:HB2	3:F:495:TRP:HA	1.64	0.80
1:C:540:LEU:HD22	1:C:545:TRP:CZ2	2.16	0.80
1:C:522:LYS:O	1:C:526:THR:HG22	1.80	0.80
3:E:490:ASN:OD1	3:E:495:TRP:HB2	1.81	0.80
1:C:666:ASP:OD1	1:C:666:ASP:N	2.15	0.79
2:D:45:CYS:SG	2:D:47:ASN:HB2	2.21	0.79
3:E:163:LYS:O	3:E:168:MET:N	2.16	0.79
3:E:170:ASP:OD1	3:E:170:ASP:N	2.15	0.79
3:F:213:PHE:CD2	3:F:282:LEU:CD1	2.66	0.79
1:A:611:LEU:O	2:B:22:PHE:CE2	2.35	0.79
1:C:625:LEU:O	1:C:629:THR:HG22	1.82	0.78
3:F:254:PRO:HB2	3:F:256:PRO:HD2	1.64	0.78
3:E:482:VAL:O	3:E:582:LYS:NZ	2.16	0.78
3:E:487:GLU:HA	3:E:495:TRP:NE1	1.98	0.78
3:E:251:ILE:HG22	3:E:252:GLY:H	1.49	0.77
3:E:255:PHE:N	3:E:256:PRO:CD	2.48	0.77
3:E:520:TYR:HB3	3:E:562:LEU:HD21	1.65	0.77
3:E:456:LEU:HB3	3:E:459:GLY:HA3	1.67	0.76
3:F:326:ARG:HH11	3:F:326:ARG:HB3	1.50	0.76
3:F:213:PHE:HD2	3:F:282:LEU:CD1	1.98	0.76
1:A:450:MET:HE1	1:A:492:LEU:HD23	1.68	0.76
1:C:563:TYR:OH	3:F:463:ASP:OD2	2.04	0.76
1:C:618:ASP:N	1:C:618:ASP:OD1	2.18	0.76
3:E:456:LEU:HB3	3:E:459:GLY:CA	2.15	0.75
3:E:52:GLU:O	3:E:55:LYS:CD	2.34	0.75
1:A:539:VAL:C	1:A:540:LEU:HD23	2.11	0.75
3:E:108:GLU:HG2	3:E:112:GLU:HG3	1.69	0.75
3:E:52:GLU:HB2	3:E:55:LYS:NZ	2.01	0.75
3:F:336:LEU:HD13	3:F:383:LYS:HG2	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:PHE:O	1:A:469:MET:HG2	1.86	0.75
3:F:213:PHE:HE2	3:F:282:LEU:HD11	1.50	0.75
3:E:136:LEU:HD21	3:E:139:LYS:CG	2.17	0.74
3:E:329:GLU:HG3	3:E:377:ILE:HG13	1.69	0.74
1:A:647:LYS:CB	1:A:675:TYR:CD1	2.70	0.74
3:F:291:TYR:CD2	3:F:334:LYS:HE3	2.22	0.74
3:E:105:GLY:O	3:E:108:GLU:HB3	1.87	0.74
3:E:255:PHE:HA	3:E:258:MET:HG3	1.69	0.74
1:C:467:ALA:HB2	1:C:504:LEU:HD11	1.70	0.74
3:E:368:LEU:O	3:E:372:MET:HG3	1.87	0.74
1:C:534:ASP:HB3	2:D:26:LYS:HG2	1.68	0.74
1:A:535:PHE:CE2	1:A:562:SER:HB3	2.23	0.73
3:E:398:GLN:HB2	3:E:440:TRP:CE2	2.22	0.73
3:E:487:GLU:HA	3:E:495:TRP:CD1	2.23	0.73
3:F:447:ILE:HD12	3:F:497:GLU:HG3	1.70	0.73
3:F:455:PHE:CE2	3:F:457:PRO:HB3	2.23	0.73
3:E:413:HIS:HD2	3:E:415:GLY:H	1.36	0.73
2:B:46:ARG:HD2	3:E:472:MET:HB3	1.68	0.73
1:C:524:HIS:HD1	1:C:524:HIS:C	1.97	0.73
1:C:428:SER:HA	1:C:431:LYS:HD3	1.70	0.72
3:F:107:LEU:HD12	3:F:149:THR:HG21	1.71	0.72
3:F:461:GLU:HG2	3:F:515:MET:HE3	1.71	0.72
3:F:54:ASN:O	3:F:58:ILE:HG13	1.90	0.72
1:C:528:SER:HB2	3:F:527:SER:O	1.90	0.72
2:D:34:ALA:HB1	3:F:373:THR:HG22	1.72	0.72
1:C:493:LYS:NZ	1:C:498:PHE:HD1	1.88	0.71
2:B:49:ILE:HG23	2:B:50:MET:HG2	1.71	0.71
3:F:166:ILE:HG13	3:F:168:MET:HG2	1.71	0.71
3:F:218:CYS:HB3	3:F:219:PRO:HD3	1.71	0.71
1:C:593:ASN:OD1	1:C:598:ARG:NH1	2.23	0.71
3:F:13:CYS:HA	3:F:16:LEU:HD12	1.73	0.70
1:C:515:LYS:NZ	1:C:538:GLN:OE1	2.23	0.70
3:E:255:PHE:CE1	3:E:303:LEU:HD13	2.25	0.70
3:E:462:THR:CG2	3:E:467:ASN:ND2	2.53	0.70
3:F:497:GLU:O	3:F:501:ILE:HG12	1.92	0.70
1:C:523:LYS:HA	1:C:526:THR:HG21	1.74	0.70
1:C:593:ASN:ND2	2:D:20:LYS:O	2.24	0.70
3:F:201:ASN:N	3:F:201:ASN:OD1	2.25	0.70
3:E:61:MET:O	3:E:64:ASN:ND2	2.25	0.69
1:A:643:LEU:HB3	1:A:649:LEU:HD12	1.75	0.69
1:C:523:LYS:C	1:C:526:THR:HG23	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:50:GLN:O	3:E:51:ASN:HB2	1.91	0.69
3:E:462:THR:HG22	3:E:467:ASN:ND2	2.07	0.69
1:A:621:THR:HG23	1:A:624:GLN:OE1	1.92	0.69
2:D:79:PHE:HZ	2:D:96:LEU:HD13	1.57	0.69
2:D:52:LEU:HD12	2:D:52:LEU:H	1.57	0.69
1:C:629:THR:HG23	1:C:631:ILE:H	1.56	0.69
3:E:486:ASN:C	3:E:495:TRP:HE1	2.01	0.69
3:F:213:PHE:O	3:F:285:SER:OG	2.11	0.69
3:F:217:LYS:HE3	3:F:281:GLN:OE1	1.93	0.69
1:A:539:VAL:O	1:A:540:LEU:HD23	1.93	0.69
2:D:41:ASN:HB2	2:D:47:ASN:O	1.94	0.68
3:F:553:MET:O	3:F:556:LYS:HG2	1.93	0.68
2:D:53:CYS:HB3	2:D:68:CYS:SG	2.33	0.68
3:F:513:LEU:HD13	3:F:569:GLU:HG2	1.74	0.68
1:A:493:LYS:HA	1:A:501:THR:HG21	1.75	0.68
2:D:66:GLU:HG3	2:D:67:GLU:HG2	1.75	0.68
3:F:46:LEU:CD2	3:F:85:VAL:CG2	2.71	0.68
3:F:401:TYR:OH	3:F:445:GLN:O	2.11	0.68
3:F:46:LEU:O	3:F:50:GLN:CD	2.37	0.68
3:F:362:LEU:O	3:F:366:GLN:HG3	1.93	0.68
1:A:577:ARG:HD3	2:B:33:TRP:CE3	2.28	0.68
1:C:558:GLU:HB3	2:D:24:VAL:HG21	1.75	0.68
3:E:136:LEU:CD2	3:E:139:LYS:HG3	2.24	0.67
1:C:634:ASP:OD1	1:C:634:ASP:N	2.24	0.67
3:E:258:MET:HB2	3:E:286:MET:HE1	1.77	0.67
3:F:294:PHE:O	3:F:341:ASN:ND2	2.26	0.67
1:A:614:TYR:HB2	2:B:22:PHE:HE2	1.59	0.67
3:F:14:GLN:HE21	3:F:54:ASN:HD21	1.42	0.67
3:F:161:TYR:HB2	3:F:224:GLN:HE21	1.58	0.67
3:E:57:ILE:O	3:E:61:MET:N	2.28	0.66
3:E:255:PHE:HE1	3:E:303:LEU:CD1	2.06	0.66
3:E:309:PRO:HA	3:E:312:LEU:HD12	1.77	0.66
3:F:148:SER:O	3:F:152:ASN:ND2	2.27	0.66
3:F:385:LEU:HD11	3:F:419:PHE:CE2	2.31	0.66
1:A:611:LEU:O	2:B:22:PHE:CD2	2.49	0.66
1:A:646:SER:OG	1:A:648:LEU:CD1	2.30	0.66
1:C:628:SER:OG	1:C:629:THR:N	2.26	0.66
1:C:476:HIS:O	1:C:478:ASN:ND2	2.29	0.66
1:C:527:ASN:ND2	3:F:551:PRO:CG	2.58	0.66
2:D:67:GLU:HG3	2:D:68:CYS:N	2.09	0.66
3:E:487:GLU:O	3:E:488:ASN:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:351:LEU:HB3	3:E:395:LEU:HA	1.78	0.65
1:A:486:ALA:HB2	1:A:508:PHE:CZ	2.32	0.65
1:C:524:HIS:CD2	1:C:569:PHE:HD1	2.11	0.65
3:F:126:LEU:HD13	3:F:183:PHE:HB2	1.77	0.65
3:E:43:ASP:OD1	3:E:43:ASP:N	2.21	0.65
3:F:505:PHE:O	3:F:509:LEU:HB2	1.97	0.65
3:E:486:ASN:O	3:E:495:TRP:NE1	2.27	0.65
1:A:669:ILE:N	1:A:669:ILE:HD12	2.12	0.64
3:E:567:LEU:O	3:E:570:SER:OG	2.14	0.64
3:E:255:PHE:HB2	3:E:289:LEU:HD21	1.79	0.64
3:E:255:PHE:CZ	3:E:303:LEU:HD13	2.33	0.64
3:E:280:LYS:O	3:E:281:GLN:NE2	2.31	0.64
3:E:255:PHE:HE1	3:E:303:LEU:HD11	1.59	0.64
3:F:280:LYS:H	3:F:280:LYS:HD2	1.62	0.64
3:F:291:TYR:CE2	3:F:334:LYS:HE3	2.33	0.64
3:F:356:LEU:HA	3:F:361:PHE:HB2	1.79	0.64
3:F:480:TYR:CZ	3:F:484:LYS:HG3	2.32	0.64
2:B:94:CYS:HB2	2:B:101:TRP:HE3	1.63	0.64
3:F:352:LEU:HD12	3:F:396:ASP:OD1	1.97	0.63
1:C:493:LYS:NZ	1:C:501:THR:OG1	2.32	0.63
1:C:530:PRO:O	1:C:561:ARG:NH1	2.30	0.63
3:E:457:PRO:O	3:E:458:GLU:C	2.39	0.63
3:E:286:MET:HE1	3:E:289:LEU:HD23	1.79	0.63
3:E:462:THR:CG2	3:E:467:ASN:HD22	2.12	0.63
3:E:14:GLN:HB2	3:E:54:ASN:ND2	2.14	0.63
3:E:362:LEU:C	3:E:365:PRO:HD2	2.24	0.63
1:C:498:PHE:CZ	1:C:502:SER:HA	2.34	0.63
3:E:416:VAL:O	3:E:420:ILE:HG12	1.98	0.62
3:F:444:PRO:HA	3:F:447:ILE:HG12	1.81	0.62
1:C:493:LYS:HZ2	1:C:498:PHE:HD1	1.47	0.62
3:E:490:ASN:ND2	3:E:492:THR:O	2.31	0.62
3:F:181:ILE:HG21	3:F:243:GLU:HG2	1.81	0.62
3:F:439:LYS:HB2	3:F:442:THR:CG2	2.29	0.62
3:E:258:MET:HB2	3:E:286:MET:CE	2.28	0.62
3:E:188:VAL:HG11	3:E:247:PHE:CE1	2.35	0.62
3:E:413:HIS:O	3:E:417:GLU:HG3	1.99	0.62
3:F:203:LYS:O	3:F:207:GLU:HG2	1.99	0.62
1:A:668:LEU:C	1:A:669:ILE:HD12	2.25	0.62
3:F:326:ARG:HH11	3:F:326:ARG:CB	2.12	0.61
2:D:87:TRP:CD1	2:D:87:TRP:C	2.78	0.61
3:E:218:CYS:HB3	3:E:219:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:431:SER:O	3:F:432:LEU:HD23	2.00	0.61
3:E:67:GLY:O	3:E:71:ARG:HG3	2.00	0.61
3:F:255:PHE:CG	3:F:256:PRO:HD3	2.36	0.61
2:D:55:GLU:O	2:D:59:ASN:ND2	2.34	0.61
3:E:490:ASN:CG	3:E:495:TRP:HD1	2.08	0.61
3:F:457:PRO:HG2	3:F:458:GLU:HG3	1.82	0.61
3:F:557:VAL:HG23	3:F:558:LEU:HD23	1.82	0.61
2:B:54:ILE:HG23	2:B:55:GLU:N	2.16	0.60
3:E:109:LEU:O	3:E:113:PRO:HD2	2.01	0.60
3:E:46:LEU:HD21	3:E:88:LEU:HD13	1.83	0.60
3:E:136:LEU:HD23	3:E:139:LYS:HB2	1.82	0.60
3:E:369:VAL:HA	3:E:372:MET:SD	2.40	0.60
3:E:487:GLU:CA	3:E:495:TRP:NE1	2.63	0.60
3:E:487:GLU:N	3:E:495:TRP:CE2	2.70	0.60
1:C:527:ASN:HD22	3:F:551:PRO:CG	2.14	0.60
3:E:487:GLU:N	3:E:495:TRP:CZ2	2.69	0.60
1:A:583:TYR:O	1:A:586:SER:N	2.23	0.60
3:E:177:CYS:HB3	3:E:240:PHE:CD1	2.37	0.60
3:E:502:GLU:HA	3:E:506:LEU:HB2	1.82	0.60
2:B:49:ILE:O	2:B:50:MET:HB2	2.01	0.60
1:C:540:LEU:HD13	1:C:545:TRP:CD2	2.37	0.60
3:F:115:GLY:N	3:F:118:ILE:HG13	2.17	0.60
3:F:377:ILE:HG22	3:F:379:THR:HG23	1.83	0.60
1:C:629:THR:OG1	1:C:631:ILE:HG13	2.02	0.60
3:F:105:GLY:O	3:F:108:GLU:HB3	2.02	0.60
3:F:113:PRO:HB2	3:F:117:GLN:HB3	1.82	0.60
1:A:642:ILE:HD11	1:A:688:MET:HA	1.85	0.59
3:E:317:MET:HG3	3:E:361:PHE:CE1	2.38	0.59
3:F:115:GLY:H	3:F:118:ILE:HG13	1.68	0.59
3:F:161:TYR:HB2	3:F:224:GLN:NE2	2.18	0.59
1:A:686:VAL:HG22	1:A:687:PRO:O	2.03	0.59
2:B:53:CYS:HB3	2:B:68:CYS:SG	2.42	0.59
1:C:588:GLY:HA3	1:C:608:MET:HE1	1.85	0.59
3:F:178:LYS:NZ	3:F:236:PRO:HB3	2.17	0.59
3:F:46:LEU:HD22	3:F:85:VAL:CG2	2.31	0.58
3:F:46:LEU:O	3:F:50:GLN:NE2	2.36	0.58
2:B:90:THR:OG1	2:B:91:ARG:NE	2.37	0.58
3:E:376:PRO:HB2	3:E:377:ILE:HD13	1.84	0.58
3:E:406:CYS:C	3:E:410:THR:HG22	2.28	0.58
3:E:407:LEU:HA	3:E:410:THR:CG2	2.33	0.58
3:E:456:LEU:HB3	3:E:459:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:PHE:CZ	1:A:525:LEU:HD11	2.38	0.58
1:C:508:PHE:O	1:C:511:ILE:HG12	2.02	0.58
3:E:110:ILE:HG23	3:E:111:GLU:H	1.68	0.58
1:C:528:SER:HB2	3:F:531:GLN:HG2	1.85	0.58
3:F:17:GLU:O	3:F:18:GLU:HB3	2.04	0.58
3:F:213:PHE:CD2	3:F:282:LEU:HD11	2.35	0.58
3:E:52:GLU:HB2	3:E:55:LYS:HZ3	1.69	0.58
3:F:326:ARG:HH11	3:F:326:ARG:CG	2.16	0.58
1:C:535:PHE:CD1	1:C:536:SER:N	2.72	0.58
3:F:160:PRO:HB2	3:F:166:ILE:HG23	1.86	0.58
3:E:110:ILE:HG23	3:E:111:GLU:N	2.19	0.58
2:B:48:HIS:HB3	2:B:51:ASP:HB2	1.85	0.57
3:F:310:LEU:HD21	3:F:355:TYR:CE1	2.39	0.57
3:E:320:ILE:HD13	3:E:339:LEU:HB2	1.85	0.57
3:E:462:THR:HG21	3:E:467:ASN:ND2	2.18	0.57
1:A:535:PHE:HE2	1:A:562:SER:HB3	1.67	0.57
1:C:528:SER:HB3	3:F:531:GLN:HB3	1.87	0.57
3:E:133:ILE:HD13	3:E:143:ILE:HG13	1.86	0.57
1:C:474:LEU:HD22	1:C:511:ILE:HD13	1.85	0.57
1:C:523:LYS:CA	1:C:526:THR:CG2	2.79	0.57
3:E:251:ILE:HG22	3:E:252:GLY:N	2.18	0.57
3:F:293:VAL:HG12	3:F:294:PHE:CD1	2.39	0.57
1:C:642:ILE:HD13	1:C:686:VAL:HG23	1.85	0.57
1:C:527:ASN:ND2	3:F:551:PRO:HD3	2.19	0.57
1:C:574:HIS:HB3	1:C:577:ARG:HD3	1.87	0.57
3:E:168:MET:O	3:E:168:MET:HG3	2.04	0.57
1:A:483:ASP:OD2	1:A:483:ASP:N	2.37	0.57
1:A:536:SER:OG	2:B:28:ASN:ND2	2.38	0.57
3:E:100:LYS:O	3:E:104:LEU:HD12	2.04	0.57
3:E:453:VAL:HG23	3:E:454:LEU:HG	1.87	0.57
3:F:279:ASN:ND2	3:F:279:ASN:O	2.38	0.57
3:F:110:ILE:HG23	3:F:153:GLN:NE2	2.19	0.57
3:E:44:GLN:HA	3:E:47:GLU:HB3	1.86	0.57
3:F:495:TRP:N	3:F:495:TRP:CD1	2.73	0.57
3:E:486:ASN:C	3:E:495:TRP:NE1	2.63	0.57
1:C:484:ALA:HA	1:C:487:SER:HB3	1.87	0.56
3:F:286:MET:HB3	3:F:319:HIS:HE1	1.70	0.56
3:F:351:LEU:O	3:F:396:ASP:N	2.38	0.56
3:F:356:LEU:HA	3:F:361:PHE:CB	2.34	0.56
2:B:94:CYS:HB2	2:B:101:TRP:CE3	2.40	0.56
3:E:494:LEU:HD13	3:E:495:TRP:N	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:137:HIS:CG	3:F:138:ASN:N	2.73	0.56
1:C:528:SER:CB	3:F:531:GLN:HG2	2.34	0.56
3:E:494:LEU:CD1	3:E:494:LEU:C	2.77	0.56
2:D:66:GLU:HG3	2:D:67:GLU:H	1.70	0.56
1:C:503:LYS:HD2	1:C:544:SER:HA	1.87	0.56
3:E:254:PRO:HB2	3:E:256:PRO:HD2	1.87	0.56
1:C:510:ASP:O	1:C:514:SER:OG	2.22	0.56
2:D:77:HIS:CE1	2:D:97:ASP:OD1	2.58	0.56
1:C:507:MET:HG2	1:C:545:TRP:CE2	2.40	0.56
1:C:524:HIS:C	1:C:524:HIS:ND1	2.58	0.56
3:E:487:GLU:CA	3:E:495:TRP:CE2	2.88	0.56
3:F:279:ASN:HD22	3:F:280:LYS:N	2.02	0.56
3:F:392:ILE:O	3:F:400:LYS:NZ	2.38	0.56
1:C:621:THR:HG23	1:C:624:GLN:OE1	2.06	0.56
3:E:353:TYR:N	3:E:396:ASP:OD2	2.39	0.56
3:F:367:GLY:O	3:F:371:VAL:HG23	2.05	0.56
1:A:532:ASP:OD1	1:A:532:ASP:N	2.31	0.56
1:A:528:SER:OG	3:E:527:SER:OG	2.14	0.55
1:A:444:ASP:OD2	1:A:448:GLN:NE2	2.40	0.55
1:C:661:VAL:HG13	1:C:662:GLU:N	2.20	0.55
3:F:460:ALA:HB1	3:F:515:MET:CE	2.31	0.55
3:F:531:GLN:O	3:F:532:LYS:HE3	2.06	0.55
3:E:377:ILE:HD13	3:E:377:ILE:N	2.22	0.55
3:F:5:GLU:OE1	3:F:35:ARG:NH1	2.38	0.55
3:E:51:ASN:O	3:E:52:GLU:HG2	2.05	0.55
1:A:450:MET:HE2	1:A:491:LYS:HB3	1.89	0.55
3:F:180:LEU:O	3:F:184:THR:OG1	2.23	0.55
1:A:597:ASN:HD22	1:C:657:ASN:HD21	1.55	0.55
3:E:107:LEU:O	3:E:110:ILE:HG22	2.07	0.55
2:D:46:ARG:O	3:F:422:GLN:NE2	2.40	0.55
3:E:80:ASP:H	3:E:83:ARG:HE	1.55	0.55
3:E:490:ASN:OD1	3:E:495:TRP:CB	2.54	0.55
3:F:256:PRO:O	3:F:257:LYS:HB2	2.07	0.55
3:F:320:ILE:CD1	3:F:339:LEU:HA	2.37	0.55
3:F:485:ASP:OD2	3:F:492:THR:OG1	2.23	0.55
3:F:140:ALA:HA	3:F:143:ILE:HD12	1.88	0.54
1:A:582:LEU:HD11	2:B:32:LEU:HG	1.90	0.54
1:A:612:LEU:HD23	2:B:22:PHE:CB	2.37	0.54
3:F:528:GLN:O	3:F:531:GLN:HG3	2.07	0.54
1:C:589:GLU:OE1	2:D:26:LYS:HD3	2.07	0.54
3:E:181:ILE:HG21	3:E:243:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:510:HIS:NE2	3:E:576:GLU:OE1	2.24	0.54
3:F:181:ILE:HD11	3:F:240:PHE:CD1	2.42	0.54
1:A:607:GLN:HG2	1:A:643:LEU:HD21	1.90	0.54
1:C:488:MET:O	1:C:492:LEU:HB2	2.07	0.54
1:C:444:ASP:O	1:C:447:ASN:ND2	2.41	0.54
1:C:540:LEU:HB3	1:C:545:TRP:CD1	2.41	0.54
3:F:151:TRP:NE1	3:F:214:LYS:HB3	2.22	0.54
2:D:93:VAL:HG22	2:D:94:CYS:H	1.73	0.54
3:F:427:GLN:O	3:F:431:SER:OG	2.21	0.54
1:C:558:GLU:N	1:C:558:GLU:OE1	2.40	0.54
3:E:45:LEU:HD22	3:E:89:ILE:HD11	1.90	0.54
2:D:47:ASN:ND2	2:D:54:ILE:HA	2.22	0.53
3:E:405:ARG:NH2	3:E:448:SER:OG	2.41	0.53
3:E:417:GLU:O	3:E:421:ILE:HG13	2.08	0.53
3:F:247:PHE:O	3:F:251:ILE:HD13	2.08	0.53
1:A:647:LYS:NZ	1:A:676:LYS:O	2.22	0.53
2:B:53:CYS:HA	2:B:80:HIS:CE1	2.43	0.53
2:D:79:PHE:CZ	2:D:96:LEU:HD13	2.41	0.53
1:A:602:GLN:HB2	1:A:683:ASN:HA	1.90	0.53
1:C:527:ASN:ND2	3:F:551:PRO:CD	2.72	0.53
1:C:664:LYS:HB2	1:C:667:THR:HG23	1.90	0.53
2:B:94:CYS:SG	2:B:95:PRO:HD2	2.48	0.53
3:E:160:PRO:O	3:E:161:TYR:CD1	2.62	0.53
3:F:99:PRO:O	3:F:103:LEU:HB2	2.09	0.53
3:F:242:SER:HB2	3:F:298:ILE:HD13	1.91	0.53
1:A:427:ASP:HB2	1:A:473:ARG:HE	1.74	0.53
3:F:406:CYS:O	3:F:410:THR:OG1	2.26	0.53
1:A:535:PHE:CD2	1:A:562:SER:HB3	2.44	0.53
2:B:62:SER:H	2:B:65:SER:HB2	1.74	0.53
3:E:326:ARG:NH1	3:E:328:GLU:OE2	2.41	0.53
3:E:413:HIS:CD2	3:E:415:GLY:H	2.22	0.53
3:F:6:LEU:HB2	3:F:32:ALA:HB1	1.90	0.53
3:F:507:LYS:N	3:F:508:PRO:HD2	2.24	0.53
1:C:507:MET:HG2	1:C:545:TRP:CD2	2.44	0.53
3:F:170:ASP:OD2	3:F:170:ASP:N	2.42	0.53
2:D:94:CYS:HB3	2:D:97:ASP:HB2	1.90	0.52
3:F:104:LEU:HA	3:F:107:LEU:HB2	1.90	0.52
1:A:621:THR:OG1	1:A:624:GLN:HG3	2.09	0.52
2:D:36:ASP:OD1	2:D:37:ILE:N	2.42	0.52
1:C:493:LYS:NZ	1:C:498:PHE:CD1	2.75	0.52
3:E:92:LEU:O	3:E:96:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:47:GLU:O	3:F:50:GLN:HG2	2.10	0.52
3:F:74:LEU:HD21	3:F:124:LEU:HD22	1.92	0.52
1:A:429:LEU:HG	1:A:430:LEU:N	2.22	0.52
3:E:199:LEU:HD12	3:E:202:GLU:HB2	1.90	0.52
3:E:499:GLY:O	3:E:502:GLU:HG2	2.09	0.52
3:E:576:GLU:HA	3:E:579:ILE:HB	1.92	0.52
3:F:303:LEU:HG	3:F:304:PRO:HD2	1.92	0.52
3:F:362:LEU:C	3:F:365:PRO:HD2	2.35	0.52
3:F:439:LYS:HB2	3:F:442:THR:HG21	1.91	0.52
3:F:154:LEU:HD12	3:F:155:SER:N	2.25	0.52
3:F:375:CYS:O	3:F:381:ARG:HD3	2.09	0.52
1:A:426:CYS:O	1:A:430:LEU:HB2	2.10	0.52
3:F:121:SER:O	3:F:125:LEU:HB2	2.08	0.52
3:F:72:CYS:HG	3:F:86:TYR:HE2	1.55	0.52
3:F:213:PHE:HD2	3:F:282:LEU:HD12	1.73	0.52
3:F:255:PHE:CD2	3:F:256:PRO:HD3	2.45	0.52
3:F:328:GLU:OE2	3:F:328:GLU:N	2.32	0.52
1:A:426:CYS:HA	1:A:429:LEU:HD23	1.91	0.52
3:E:300:ILE:HG12	3:E:300:ILE:O	2.10	0.52
3:F:293:VAL:O	3:F:300:ILE:HD11	2.09	0.52
3:F:447:ILE:HD11	3:F:493:GLY:HA2	1.92	0.52
3:E:346:ILE:HG22	3:E:347:GLU:O	2.09	0.51
3:E:490:ASN:OD1	3:E:495:TRP:CG	2.63	0.51
3:F:443:GLY:O	3:F:446:LEU:N	2.29	0.51
3:F:479:ARG:O	3:F:483:ILE:HG13	2.10	0.51
2:B:58:ALA:HB2	3:E:480:TYR:CD1	2.45	0.51
1:A:537:ILE:HG21	1:A:566:PHE:CZ	2.45	0.51
1:A:671:LEU:HD12	1:A:672:TYR:N	2.25	0.51
3:E:258:MET:CB	3:E:286:MET:CE	2.88	0.51
3:F:178:LYS:HZ3	3:F:236:PRO:HB3	1.75	0.51
3:F:255:PHE:O	3:F:258:MET:HB2	2.09	0.51
1:A:647:LYS:CB	1:A:675:TYR:HD1	2.23	0.51
3:E:66:VAL:HG23	3:E:93:LEU:HD13	1.91	0.51
3:E:195:LYS:HG2	3:E:196:GLU:N	2.26	0.51
3:E:413:HIS:HB3	3:E:416:VAL:HG13	1.91	0.51
2:B:40:ASP:HB2	2:B:48:HIS:CE1	2.46	0.51
1:C:540:LEU:HD22	1:C:545:TRP:CE2	2.45	0.51
1:C:559:LEU:HD13	2:D:27:TRP:CE2	2.45	0.51
1:A:507:MET:HE3	1:A:544:SER:O	2.10	0.51
3:E:125:LEU:C	3:E:128:PRO:HD2	2.36	0.51
3:F:329:GLU:HG3	3:F:380:LEU:CD1	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:388:LEU:O	3:F:392:ILE:HG13	2.11	0.51
1:C:481:SER:OG	1:C:484:ALA:N	2.43	0.50
1:C:527:ASN:ND2	3:F:551:PRO:CB	2.55	0.50
1:C:621:THR:HG23	1:C:624:GLN:CD	2.37	0.50
2:D:72:TRP:CD2	2:D:78:ALA:HB2	2.46	0.50
3:E:450:LEU:HA	3:E:453:VAL:HG22	1.94	0.50
3:F:95:LYS:O	3:F:135:LYS:NZ	2.42	0.50
1:A:621:THR:HG23	1:A:624:GLN:CD	2.37	0.50
3:E:494:LEU:O	3:E:497:GLU:N	2.45	0.50
3:F:30:GLN:HG3	3:F:64:ASN:HB3	1.94	0.50
3:E:507:LYS:N	3:E:508:PRO:HD2	2.27	0.50
3:F:129:LEU:O	3:F:133:ILE:HG13	2.12	0.50
3:F:220:LEU:HD13	3:F:292:LEU:HD11	1.94	0.50
3:E:238:ARG:HG3	3:E:298:ILE:HD11	1.93	0.50
3:E:413:HIS:HD2	3:E:415:GLY:N	2.06	0.50
1:C:492:LEU:C	1:C:492:LEU:HD13	2.37	0.50
3:E:424:ILE:O	3:E:428:ILE:HG13	2.11	0.50
1:C:530:PRO:C	1:C:561:ARG:HH22	2.06	0.50
3:F:323:PHE:HD1	3:F:331:VAL:HG12	1.76	0.50
3:E:10:ILE:HD11	3:E:29:PHE:HE1	1.77	0.49
3:E:177:CYS:O	3:E:181:ILE:HG12	2.12	0.49
1:A:626:THR:CG2	1:A:636:LEU:HD23	2.36	0.49
1:C:588:GLY:CA	1:C:608:MET:HE1	2.41	0.49
3:E:90:PHE:O	3:E:94:VAL:HG13	2.12	0.49
3:F:17:GLU:O	3:F:18:GLU:OE2	2.30	0.49
3:F:299:HIS:HB3	3:F:302:GLN:HG3	1.94	0.49
1:A:535:PHE:CD1	1:A:535:PHE:C	2.89	0.49
3:F:352:LEU:O	3:F:355:TYR:HD2	1.95	0.49
1:C:527:ASN:O	1:C:529:GLU:HG2	2.12	0.49
3:E:577:GLU:O	3:E:581:ILE:HD13	2.12	0.49
3:F:63:TRP:O	3:F:66:VAL:HG12	2.11	0.49
3:F:130:GLN:OE1	3:F:183:PHE:HA	2.12	0.49
3:F:424:ILE:O	3:F:428:ILE:HG13	2.13	0.49
2:B:58:ALA:HB2	3:E:480:TYR:HD1	1.78	0.49
2:B:62:SER:H	2:B:65:SER:CB	2.25	0.49
3:F:478:LEU:HD12	3:F:575:VAL:HG11	1.94	0.49
1:C:540:LEU:O	2:D:32:LEU:HA	2.13	0.49
2:B:88:LEU:HD11	2:B:101:TRP:CD1	2.48	0.49
1:C:623:GLN:O	1:C:626:THR:HG22	2.13	0.49
3:E:375:CYS:HA	3:E:376:PRO:HD3	1.72	0.49
1:A:582:LEU:HB3	1:A:584:GLN:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:HIS:HD2	1:C:569:PHE:CD1	2.16	0.49
3:E:520:TYR:CB	3:E:562:LEU:HD21	2.38	0.49
3:F:339:LEU:O	3:F:342:SER:HB2	2.13	0.49
1:C:471:ALA:O	1:C:475:VAL:HG12	2.12	0.49
3:E:118:ILE:HG22	3:E:119:SER:N	2.28	0.49
3:F:73:LEU:HD22	3:F:87:PHE:CE2	2.47	0.49
2:B:87:TRP:CE2	2:B:95:PRO:HB3	2.49	0.48
2:D:47:ASN:HD22	2:D:54:ILE:HA	1.77	0.48
3:F:249:SER:HB3	3:F:302:GLN:HE22	1.78	0.48
3:F:143:ILE:HD13	3:F:204:LEU:HD13	1.93	0.48
3:F:351:LEU:HB3	3:F:395:LEU:HA	1.94	0.48
1:A:612:LEU:HD23	2:B:22:PHE:HB3	1.95	0.48
1:A:662:GLU:O	1:A:662:GLU:HG2	2.13	0.48
1:C:527:ASN:ND2	3:F:551:PRO:HG3	2.27	0.48
3:F:66:VAL:HG21	3:F:106:LEU:HD23	1.95	0.48
3:F:107:LEU:O	3:F:110:ILE:HG13	2.13	0.48
3:F:466:GLN:HE21	3:F:466:GLN:HA	1.79	0.48
3:F:512:GLY:O	3:F:516:SER:OG	2.31	0.48
3:E:365:PRO:O	3:E:368:LEU:HB2	2.13	0.48
3:F:414:SER:OG	3:F:467:ASN:HA	2.13	0.48
1:A:521:PHE:CE2	1:A:525:LEU:HD11	2.49	0.48
3:E:53:LYS:HA	3:E:54:ASN:HA	1.58	0.48
3:E:532:LYS:HG2	3:E:533:SER:N	2.28	0.48
3:E:106:LEU:HD22	3:E:125:LEU:HD23	1.94	0.48
3:E:254:PRO:CB	3:E:256:PRO:HD2	2.43	0.48
3:E:487:GLU:HA	3:E:495:TRP:CE2	2.48	0.48
2:D:25:LYS:HG2	2:D:26:LYS:HG3	1.96	0.48
3:E:254:PRO:HB2	3:E:256:PRO:CD	2.44	0.48
1:A:616:THR:OG1	1:A:620:TYR:OH	2.26	0.48
1:A:688:MET:HE3	1:A:688:MET:HB2	1.74	0.48
3:E:45:LEU:HD22	3:E:89:ILE:CD1	2.44	0.48
3:E:52:GLU:HB2	3:E:55:LYS:HZ2	1.79	0.48
1:A:553:PHE:CD1	1:A:606:PHE:HE1	2.31	0.47
1:A:561:ARG:O	1:A:562:SER:C	2.56	0.47
1:A:572:SER:OG	3:E:557:VAL:HB	2.14	0.47
1:A:611:LEU:O	2:B:22:PHE:HE2	1.93	0.47
1:A:470:LEU:HG	1:A:474:LEU:HD22	1.95	0.47
2:B:49:ILE:O	2:B:50:MET:CB	2.60	0.47
3:E:414:SER:HB2	3:E:469:ASP:OD1	2.14	0.47
3:E:487:GLU:N	3:E:495:TRP:NE1	2.62	0.47
3:F:450:LEU:O	3:F:453:VAL:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:PRO:O	1:A:559:LEU:N	2.42	0.47
1:C:545:TRP:HA	1:C:546:PRO:HD3	1.68	0.47
3:F:34:GLN:HE21	3:F:34:GLN:HB3	1.56	0.47
3:F:398:GLN:HB2	3:F:440:TRP:CE2	2.49	0.47
3:F:550:PRO:O	3:F:553:MET:HB2	2.15	0.47
1:A:482:ASP:OD1	1:A:482:ASP:N	2.47	0.47
1:A:524:HIS:HD2	3:E:554:GLN:OE1	1.97	0.47
1:C:540:LEU:HB3	1:C:545:TRP:NE1	2.29	0.47
3:E:328:GLU:O	3:E:332:ILE:HD12	2.13	0.47
3:E:550:PRO:HG2	3:E:551:PRO:HD3	1.97	0.47
1:A:540:LEU:HD13	1:A:545:TRP:CD2	2.49	0.47
3:F:9:ILE:HG23	3:F:25:ASP:OD1	2.15	0.47
3:F:109:LEU:HD12	3:F:109:LEU:C	2.40	0.47
3:F:242:SER:HA	3:F:298:ILE:HG21	1.97	0.47
3:F:326:ARG:HH12	3:F:328:GLU:CD	2.23	0.47
2:B:44:ILE:O	3:E:472:MET:HE1	2.13	0.47
1:C:501:THR:HA	1:C:504:LEU:HD23	1.97	0.47
1:C:673:LEU:N	1:C:673:LEU:HD12	2.30	0.47
2:D:72:TRP:CE3	2:D:78:ALA:HB2	2.48	0.47
3:E:168:MET:HE3	3:E:168:MET:HB2	1.80	0.47
3:E:238:ARG:NH2	3:E:296:GLN:O	2.47	0.47
3:E:378:GLU:O	3:E:379:THR:C	2.55	0.47
3:F:109:LEU:HD12	3:F:110:ILE:N	2.29	0.47
3:F:300:ILE:HG22	3:F:300:ILE:O	2.15	0.47
3:F:329:GLU:CD	3:F:377:ILE:HD12	2.40	0.47
1:A:559:LEU:HD22	2:B:27:TRP:CE3	2.50	0.47
2:D:96:LEU:N	2:D:96:LEU:HD12	2.30	0.47
3:E:41:HIS:CD2	3:E:41:HIS:H	2.32	0.47
3:E:494:LEU:HD11	3:E:495:TRP:CD2	2.50	0.47
3:E:500:ASN:OD1	3:E:500:ASN:N	2.45	0.47
3:F:85:VAL:HG13	3:F:86:TYR:HD1	1.79	0.47
3:F:177:CYS:HB3	3:F:240:PHE:CE1	2.50	0.47
1:A:613:GLN:O	1:A:620:TYR:HE2	1.98	0.47
1:C:535:PHE:CD1	1:C:535:PHE:C	2.93	0.47
3:E:326:ARG:HH11	3:E:326:ARG:CG	2.28	0.47
3:F:326:ARG:CG	3:F:326:ARG:NH1	2.78	0.47
1:A:493:LYS:HA	1:A:501:THR:CG2	2.45	0.47
1:A:675:TYR:OH	1:A:677:ASN:ND2	2.47	0.47
3:F:27:GLY:O	3:F:31:LEU:HB2	2.15	0.47
2:B:54:ILE:CG2	2:B:55:GLU:N	2.77	0.46
2:D:67:GLU:CG	2:D:68:CYS:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:462:THR:HG22	3:E:467:ASN:HD22	1.75	0.46
1:A:534:ASP:HB3	2:B:26:LYS:HG2	1.97	0.46
3:E:365:PRO:HA	3:E:368:LEU:HD12	1.95	0.46
3:E:461:GLU:H	3:E:461:GLU:HG2	1.57	0.46
3:F:17:GLU:O	3:F:18:GLU:CB	2.63	0.46
3:F:151:TRP:CD1	3:F:214:LYS:HB3	2.50	0.46
3:F:320:ILE:HD11	3:F:339:LEU:HA	1.97	0.46
3:F:466:GLN:O	3:F:467:ASN:HB2	2.16	0.46
1:A:668:LEU:HD12	1:A:669:ILE:N	2.30	0.46
1:C:521:PHE:O	1:C:524:HIS:HB3	2.15	0.46
3:E:252:GLY:C	3:E:253:HIS:CG	2.94	0.46
3:E:398:GLN:HB2	3:E:440:TRP:CD2	2.51	0.46
3:F:218:CYS:CB	3:F:219:PRO:HD3	2.40	0.46
3:F:404:PHE:CD2	3:F:424:ILE:HG12	2.50	0.46
1:A:689:LYS:HE2	1:A:689:LYS:H	1.80	0.46
3:E:127:GLN:HB3	3:E:128:PRO:HD3	1.96	0.46
3:E:443:GLY:O	3:E:446:LEU:N	2.48	0.46
3:F:575:VAL:O	3:F:579:ILE:HG13	2.16	0.46
1:A:471:ALA:O	1:A:475:VAL:HG22	2.15	0.46
2:D:75:CYS:HB2	2:D:97:ASP:OD2	2.14	0.46
3:E:188:VAL:HG11	3:E:247:PHE:CD1	2.50	0.46
3:E:353:TYR:HB2	3:E:398:GLN:HG2	1.98	0.46
1:A:420:GLU:OE2	1:A:424:ARG:NH1	2.49	0.46
1:A:614:TYR:CE1	1:A:649:LEU:HD21	2.51	0.46
1:A:626:THR:HG22	1:A:636:LEU:HD22	1.96	0.46
3:E:91:ASP:O	3:E:94:VAL:HG22	2.14	0.46
3:E:336:LEU:HD13	3:E:383:LYS:HG2	1.98	0.46
3:E:407:LEU:HA	3:E:410:THR:HG23	1.97	0.46
3:F:582:LYS:HE2	3:F:582:LYS:HB3	1.47	0.46
1:A:669:ILE:N	1:A:669:ILE:CD1	2.78	0.46
3:E:125:LEU:N	3:E:125:LEU:HD12	2.31	0.46
3:E:320:ILE:HD13	3:E:339:LEU:CA	2.46	0.46
3:F:45:LEU:O	3:F:46:LEU:CB	2.64	0.46
3:F:122:ILE:HG22	3:F:126:LEU:HD23	1.98	0.46
3:F:211:PHE:O	3:F:215:SER:OG	2.34	0.46
3:E:425:LYS:HE2	3:E:425:LYS:HB3	1.62	0.46
3:E:509:LEU:HD23	3:E:572:LEU:HD22	1.98	0.46
3:F:112:GLU:O	3:F:113:PRO:O	2.33	0.46
3:F:115:GLY:H	3:F:118:ILE:H	1.62	0.46
1:A:641:GLN:HE21	1:A:641:GLN:HB3	1.42	0.46
3:F:130:GLN:O	3:F:134:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ASN:O	3:E:531:GLN:HG3	2.16	0.46
2:B:55:GLU:CD	3:E:574:ARG:HH21	2.22	0.46
2:B:42:CYS:O	2:B:45:CYS:O	2.34	0.45
3:E:133:ILE:O	3:E:136:LEU:O	2.34	0.45
3:E:255:PHE:CZ	3:E:303:LEU:CD1	2.94	0.45
3:E:320:ILE:HD13	3:E:339:LEU:CB	2.46	0.45
1:A:508:PHE:O	1:A:511:ILE:N	2.49	0.45
2:B:45:CYS:HB2	3:E:476:ASN:OD1	2.17	0.45
3:F:166:ILE:O	3:F:166:ILE:HG12	2.13	0.45
1:C:516:ASP:O	1:C:520:GLN:HG2	2.16	0.45
3:E:13:CYS:O	3:E:16:LEU:HG	2.17	0.45
3:F:45:LEU:O	3:F:46:LEU:HB2	2.16	0.45
1:A:565:ARG:HD2	1:A:565:ARG:HA	1.68	0.45
1:C:498:PHE:CE2	1:C:502:SER:HA	2.52	0.45
1:C:524:HIS:CD2	1:C:569:PHE:CD1	3.00	0.45
3:E:83:ARG:HD2	3:E:87:PHE:HE1	1.82	0.45
3:E:434:ARG:HB2	3:E:434:ARG:NH1	2.31	0.45
3:F:281:GLN:OE1	3:F:281:GLN:HA	2.16	0.45
3:F:431:SER:C	3:F:432:LEU:HD23	2.42	0.45
2:B:48:HIS:ND1	2:B:49:ILE:O	2.49	0.45
3:E:220:LEU:O	3:E:334:LYS:NZ	2.49	0.45
3:E:286:MET:CE	3:E:289:LEU:HD23	2.45	0.45
3:F:92:LEU:HD23	3:F:95:LYS:HD3	1.98	0.45
3:F:465:LEU:HD11	3:F:561:ALA:HB1	1.98	0.45
1:A:612:LEU:HD23	2:B:22:PHE:HB2	1.97	0.45
1:A:689:LYS:HE2	1:A:689:LYS:N	2.32	0.45
3:F:213:PHE:CD2	3:F:282:LEU:HD12	2.50	0.45
3:E:180:LEU:HD13	3:E:211:PHE:CZ	2.52	0.45
3:F:151:TRP:CE2	3:F:214:LYS:HB3	2.51	0.45
3:F:326:ARG:NH1	3:F:328:GLU:OE2	2.49	0.45
3:F:447:ILE:CD1	3:F:493:GLY:HA2	2.46	0.45
3:E:235:ASP:O	3:E:238:ARG:N	2.45	0.45
3:E:6:LEU:HD12	3:E:6:LEU:O	2.17	0.45
3:E:52:GLU:HB2	3:E:55:LYS:HD3	1.99	0.45
3:E:106:LEU:O	3:E:109:LEU:HD23	2.17	0.45
3:E:465:LEU:HA	3:E:465:LEU:HD22	1.61	0.45
3:E:582:LYS:HE2	3:E:582:LYS:HB3	1.86	0.45
3:F:359:LYS:O	3:F:360:SER:C	2.60	0.45
3:E:218:CYS:CB	3:E:219:PRO:HD3	2.46	0.45
3:E:359:LYS:HB3	3:E:359:LYS:HE2	1.63	0.45
3:F:116:LYS:HB3	3:F:116:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:385:LEU:HD12	3:F:385:LEU:O	2.16	0.45
1:A:523:LYS:HD2	1:A:523:LYS:HA	1.73	0.44
1:A:537:ILE:HG13	2:B:29:ALA:O	2.17	0.44
1:C:645:LYS:HD2	1:C:645:LYS:HA	1.82	0.44
2:D:90:THR:OG1	2:D:91:ARG:NH1	2.50	0.44
3:E:343:LEU:HD23	3:E:343:LEU:HA	1.79	0.44
3:E:352:LEU:HA	3:E:396:ASP:OD2	2.18	0.44
3:E:494:LEU:CD1	3:E:495:TRP:CD2	3.00	0.44
3:F:354:GLN:O	3:F:357:GLU:HB2	2.16	0.44
2:D:37:ILE:HD12	2:D:37:ILE:HA	1.59	0.44
3:E:372:MET:HE3	3:E:385:LEU:HD13	1.99	0.44
2:D:97:ASP:CB	2:D:99:ARG:H	2.30	0.44
3:E:95:LYS:O	3:E:135:LYS:NZ	2.50	0.44
3:E:148:SER:OG	3:E:214:LYS:NZ	2.51	0.44
3:F:93:LEU:O	3:F:97:CYS:HB2	2.17	0.44
3:F:166:ILE:HD11	3:F:170:ASP:H	1.81	0.44
3:F:417:GLU:O	3:F:421:ILE:HG13	2.17	0.44
3:E:212:CYS:O	3:E:216:LEU:HB2	2.16	0.44
3:F:10:ILE:O	3:F:14:GLN:HG3	2.18	0.44
3:F:47:GLU:O	3:F:48:ILE:C	2.58	0.44
3:F:56:VAL:O	3:F:59:LYS:HG3	2.16	0.44
3:F:320:ILE:HD13	3:F:339:LEU:HB2	2.00	0.44
3:F:456:LEU:HB3	3:F:459:GLY:H	1.81	0.44
2:B:75:CYS:O	2:B:76:ASN:HB2	2.18	0.44
3:E:44:GLN:H	3:E:44:GLN:HG2	1.48	0.44
3:E:217:LYS:O	3:E:221:LEU:HB2	2.17	0.44
3:F:320:ILE:HD13	3:F:339:LEU:HA	1.99	0.44
3:F:356:LEU:HD13	3:F:402:THR:HG21	1.99	0.44
3:F:439:LYS:HE2	3:F:442:THR:HG21	1.99	0.44
1:A:506:ARG:O	1:A:510:ASP:HB2	2.17	0.44
1:A:640:LEU:O	1:A:641:GLN:C	2.60	0.44
3:E:103:LEU:O	3:E:107:LEU:N	2.38	0.44
3:F:185:LYS:N	3:F:186:PRO:HD2	2.33	0.44
3:F:421:ILE:O	3:F:424:ILE:HB	2.17	0.44
3:F:514:ASN:OD1	3:F:514:ASN:N	2.51	0.44
1:A:553:PHE:CD1	1:A:606:PHE:CE1	3.06	0.44
1:A:597:ASN:HD22	1:C:657:ASN:ND2	2.13	0.44
2:B:49:ILE:HD12	2:B:49:ILE:HA	1.89	0.44
1:C:527:ASN:HD21	3:F:551:PRO:HD3	1.83	0.44
2:D:93:VAL:HG23	2:D:100:GLU:HA	1.98	0.44
3:E:57:ILE:HG22	3:E:61:MET:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:82:LYS:O	3:E:85:VAL:HG22	2.18	0.44
3:E:404:PHE:O	3:E:405:ARG:C	2.61	0.44
3:F:165:GLN:C	3:F:165:GLN:CD	2.85	0.44
3:F:364:VAL:N	3:F:365:PRO:CD	2.81	0.44
2:B:35:TRP:O	3:E:413:HIS:HE1	2.01	0.44
3:E:258:MET:CB	3:E:286:MET:HE1	2.45	0.44
1:A:478:ASN:OD1	1:A:479:SER:N	2.49	0.44
1:C:559:LEU:HD13	2:D:27:TRP:CD2	2.53	0.44
3:E:71:ARG:HE	3:E:112:GLU:CD	2.25	0.44
3:E:110:ILE:CG2	3:E:111:GLU:H	2.31	0.44
3:E:486:ASN:OD1	3:E:486:ASN:N	2.51	0.44
3:F:49:ILE:HG23	3:F:58:ILE:HD13	1.99	0.44
3:F:72:CYS:SG	3:F:86:TYR:CE2	3.11	0.44
3:F:574:ARG:NH2	3:F:578:LEU:HD21	2.33	0.44
3:E:76:LYS:HD2	3:E:76:LYS:HA	1.78	0.43
1:A:535:PHE:HE1	1:A:537:ILE:HB	1.83	0.43
1:C:623:GLN:NE2	1:C:627:ASP:OD1	2.51	0.43
3:E:421:ILE:O	3:E:422:GLN:C	2.61	0.43
3:F:140:ALA:HB2	3:F:204:LEU:HB2	2.00	0.43
3:F:465:LEU:HD13	3:F:565:PHE:CZ	2.52	0.43
3:F:495:TRP:CD1	3:F:495:TRP:H	2.35	0.43
1:C:528:SER:HB3	3:F:531:GLN:CG	2.49	0.43
1:C:661:VAL:HG22	1:C:662:GLU:H	1.83	0.43
3:E:66:VAL:CG2	3:E:93:LEU:HD13	2.49	0.43
3:E:103:LEU:HA	3:E:106:LEU:HD12	1.99	0.43
3:E:450:LEU:HA	3:E:450:LEU:HD12	1.78	0.43
1:C:525:LEU:C	1:C:529:GLU:HB2	2.22	0.43
3:E:291:TYR:CD2	3:E:334:LYS:HE3	2.54	0.43
3:F:256:PRO:C	3:F:258:MET:H	2.27	0.43
3:F:383:LYS:O	3:F:386:ALA:HB3	2.18	0.43
1:A:643:LEU:CB	1:A:649:LEU:HD12	2.45	0.43
3:E:109:LEU:O	3:E:110:ILE:C	2.61	0.43
3:E:188:VAL:O	3:E:192:ILE:HG13	2.17	0.43
3:E:525:LYS:HB3	3:E:525:LYS:HE3	1.89	0.43
3:F:353:TYR:O	3:F:354:GLN:C	2.62	0.43
1:C:558:GLU:CB	2:D:24:VAL:HG21	2.46	0.43
1:C:659:ASP:OD1	1:C:659:ASP:N	2.51	0.43
3:E:92:LEU:O	3:E:92:LEU:HD12	2.18	0.43
3:F:390:LEU:HD12	3:F:390:LEU:HA	1.67	0.43
3:F:130:GLN:HG3	3:F:187:PHE:CZ	2.54	0.43
3:F:563:PHE:O	3:F:566:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:PHE:CD1	1:A:536:SER:N	2.86	0.43
1:A:559:LEU:HD13	2:B:27:TRP:CE2	2.54	0.43
3:E:363:THR:O	3:E:366:GLN:HB2	2.18	0.43
3:E:398:GLN:HB2	3:E:440:TRP:CZ2	2.54	0.43
1:A:474:LEU:HD12	1:A:474:LEU:HA	1.74	0.43
3:F:351:LEU:HD12	3:F:351:LEU:HA	1.67	0.43
1:A:671:LEU:HD12	1:A:672:TYR:H	1.82	0.43
3:E:129:LEU:HD23	3:E:129:LEU:HA	1.68	0.43
1:A:422:LEU:H	1:A:422:LEU:HG	1.54	0.42
1:C:430:LEU:HD23	1:C:473:ARG:NH1	2.34	0.42
2:D:93:VAL:HG21	2:D:98:ASN:OD1	2.19	0.42
3:E:59:LYS:HA	3:E:96:LEU:O	2.18	0.42
3:E:180:LEU:O	3:E:184:THR:OG1	2.36	0.42
3:F:74:LEU:HD22	3:F:120:GLN:HG2	2.01	0.42
3:F:458:GLU:HB2	3:F:462:THR:HA	2.00	0.42
1:A:428:SER:HA	1:A:431:LYS:HE3	2.00	0.42
1:A:501:THR:O	1:A:504:LEU:N	2.49	0.42
1:A:540:LEU:HD13	1:A:545:TRP:CE3	2.54	0.42
2:B:87:TRP:CE2	2:B:91:ARG:HG3	2.54	0.42
3:E:138:ASN:O	3:E:200:GLU:HG2	2.19	0.42
3:E:306:VAL:HB	3:E:307:LEU:H	1.46	0.42
3:E:343:LEU:HD22	3:E:394:LYS:HG3	2.00	0.42
3:E:552:GLU:O	3:E:552:GLU:OE1	2.37	0.42
3:F:66:VAL:HG21	3:F:106:LEU:CD2	2.49	0.42
3:F:125:LEU:O	3:F:128:PRO:HG2	2.19	0.42
3:F:302:GLN:HE21	3:F:302:GLN:HB3	1.62	0.42
1:A:614:TYR:HB2	2:B:22:PHE:CE2	2.48	0.42
1:C:482:ASP:O	1:C:485:GLU:HB2	2.18	0.42
3:F:499:GLY:O	3:F:503:ASN:ND2	2.52	0.42
1:A:559:LEU:HD13	2:B:27:TRP:CZ2	2.54	0.42
1:C:467:ALA:HB2	1:C:504:LEU:CD1	2.47	0.42
1:C:478:ASN:HD22	1:C:478:ASN:N	2.17	0.42
3:E:417:GLU:OE1	3:E:470:ARG:HD2	2.19	0.42
3:F:72:CYS:SG	3:F:86:TYR:HE2	2.43	0.42
3:F:375:CYS:SG	3:F:376:PRO:HD2	2.59	0.42
3:E:395:LEU:O	3:E:400:LYS:NZ	2.51	0.42
3:E:153:GLN:HA	3:E:153:GLN:NE2	2.35	0.42
3:E:291:TYR:CZ	3:E:334:LYS:HG2	2.54	0.42
3:E:320:ILE:HD13	3:E:339:LEU:HA	2.00	0.42
3:E:391:TYR:O	3:E:392:ILE:C	2.63	0.42
3:E:520:TYR:O	3:E:524:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:139:LYS:HG2	3:F:141:TYR:HB3	2.01	0.42
1:A:677:ASN:HB3	1:A:679:LYS:O	2.20	0.42
2:B:73:GLY:HA3	2:B:101:TRP:CH2	2.55	0.42
1:C:617:GLU:HB2	1:C:620:TYR:OH	2.20	0.42
3:F:239:TYR:HE1	3:F:243:GLU:OE2	2.02	0.42
1:A:555:LEU:HA	1:A:556:PRO:HD3	1.78	0.42
1:C:486:ALA:O	1:C:490:SER:OG	2.25	0.42
1:C:629:THR:HG23	1:C:630:GLN:N	2.34	0.42
3:E:103:LEU:HD12	3:E:104:LEU:H	1.85	0.42
3:E:352:LEU:HA	3:E:352:LEU:HD23	1.69	0.42
1:A:523:LYS:O	1:A:526:THR:HB	2.20	0.42
1:C:643:LEU:O	1:C:646:SER:OG	2.36	0.42
1:C:677:ASN:ND2	1:C:682:VAL:HG11	2.35	0.42
3:E:571:VAL:O	3:E:574:ARG:HB3	2.19	0.42
3:F:177:CYS:HB3	3:F:240:PHE:CD1	2.55	0.42
3:F:363:THR:O	3:F:366:GLN:HB2	2.20	0.42
3:F:503:ASN:O	3:F:508:PRO:HD3	2.20	0.42
1:A:684:ILE:O	1:A:686:VAL:HG12	2.20	0.42
2:D:67:GLU:CG	2:D:68:CYS:N	2.76	0.42
3:E:334:LYS:O	3:E:335:GLY:C	2.63	0.42
3:E:413:HIS:CD2	3:E:413:HIS:C	2.98	0.42
3:F:166:ILE:HG13	3:F:168:MET:H	1.84	0.42
1:A:504:LEU:N	1:A:504:LEU:HD23	2.35	0.41
1:A:664:LYS:HB3	1:A:665:PRO:HD2	2.01	0.41
3:F:255:PHE:HZ	3:F:299:HIS:O	2.03	0.41
3:F:352:LEU:HA	3:F:396:ASP:OD1	2.20	0.41
3:F:477:LEU:HD12	3:F:477:LEU:O	2.20	0.41
3:F:494:LEU:CB	3:F:495:TRP:HA	2.39	0.41
3:E:181:ILE:CG2	3:E:243:GLU:HG2	2.50	0.41
3:E:372:MET:O	3:E:381:ARG:CD	2.52	0.41
3:E:453:VAL:HG23	3:E:454:LEU:N	2.34	0.41
3:F:59:LYS:HD3	3:F:60:ASN:N	2.35	0.41
3:F:256:PRO:O	3:F:257:LYS:CB	2.68	0.41
1:A:531:LEU:HD23	1:A:561:ARG:NH1	2.34	0.41
1:A:579:LEU:HA	1:A:579:LEU:HD23	1.82	0.41
1:A:631:ILE:O	1:A:632:LYS:C	2.62	0.41
2:B:94:CYS:N	2:B:99:ARG:O	2.49	0.41
1:C:633:MET:HE2	1:C:633:MET:HB3	1.79	0.41
2:D:28:ASN:OD1	2:D:28:ASN:N	2.53	0.41
3:E:108:GLU:OE1	3:E:109:LEU:CA	2.68	0.41
3:E:326:ARG:NH1	3:E:326:ARG:CG	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:248:LEU:H	3:F:248:LEU:HG	1.73	0.41
1:C:474:LEU:HD23	1:C:474:LEU:HA	1.89	0.41
3:E:83:ARG:O	3:E:86:TYR:N	2.50	0.41
3:E:143:ILE:O	3:E:144:GLY:C	2.63	0.41
3:E:258:MET:HB2	3:E:286:MET:HE2	2.03	0.41
3:E:344:LEU:HD12	3:E:344:LEU:HA	1.65	0.41
3:E:362:LEU:HD23	3:E:362:LEU:HA	1.72	0.41
3:F:463:ASP:O	3:F:466:GLN:O	2.37	0.41
1:A:477:GLN:O	1:A:478:ASN:ND2	2.53	0.41
2:B:93:VAL:HG23	2:B:94:CYS:O	2.20	0.41
1:C:520:GLN:HG3	1:C:573:ARG:NH1	2.36	0.41
3:F:301:ASP:OD1	3:F:302:GLN:HG2	2.20	0.41
3:F:310:LEU:HD21	3:F:355:TYR:CZ	2.56	0.41
1:C:449:VAL:O	1:C:452:LYS:HB2	2.20	0.41
2:D:45:CYS:HB3	2:D:83:CYS:SG	2.61	0.41
3:E:33:GLY:O	3:E:34:GLN:C	2.62	0.41
3:E:196:GLU:HG2	3:E:198:SER:HB3	2.01	0.41
3:F:312:LEU:HD23	3:F:312:LEU:HA	1.85	0.41
3:F:343:LEU:HD23	3:F:343:LEU:HA	1.83	0.41
2:B:93:VAL:HG23	2:B:94:CYS:N	2.35	0.41
1:C:672:TYR:CE2	1:C:674:GLY:C	2.99	0.41
3:E:238:ARG:HG2	3:E:238:ARG:HH11	1.86	0.41
3:E:248:LEU:HD23	3:E:248:LEU:HA	1.88	0.41
3:E:258:MET:H	3:E:258:MET:HG2	1.62	0.41
3:E:449:LEU:HD12	3:E:449:LEU:HA	1.87	0.41
1:A:459:LYS:HB3	1:A:459:LYS:HE3	1.82	0.41
1:A:478:ASN:CG	1:A:479:SER:H	2.25	0.41
1:A:507:MET:HG2	1:A:545:TRP:CE2	2.55	0.41
1:C:569:PHE:CD2	1:C:569:PHE:C	2.97	0.41
1:C:579:LEU:HA	2:D:32:LEU:O	2.21	0.41
3:E:280:LYS:C	3:E:282:LEU:H	2.29	0.41
3:F:165:GLN:C	3:F:165:GLN:OE1	2.64	0.41
3:F:244:ILE:O	3:F:247:PHE:HB2	2.20	0.41
3:F:316:ASN:OD1	3:F:338:LEU:HD21	2.20	0.41
3:F:443:GLY:HA3	3:F:444:PRO:HD2	1.88	0.41
3:F:478:LEU:HD22	3:F:478:LEU:HA	1.69	0.41
1:A:629:THR:OG1	1:A:631:ILE:HD12	2.20	0.41
1:C:446:LEU:HD23	1:C:446:LEU:HA	1.87	0.41
1:C:620:TYR:HB2	1:C:625:LEU:HD21	2.03	0.41
2:D:49:ILE:HD12	2:D:50:MET:H	1.85	0.41
3:E:180:LEU:HD23	3:E:180:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:191:VAL:HG23	3:E:201:ASN:ND2	2.36	0.41
3:F:117:GLN:OE1	3:F:120:GLN:HB3	2.21	0.41
3:F:241:ALA:O	3:F:245:ILE:HD12	2.21	0.41
3:E:351:LEU:HD12	3:E:351:LEU:HA	1.87	0.41
3:E:494:LEU:CD1	3:E:495:TRP:CG	3.04	0.41
1:A:477:GLN:O	1:A:478:ASN:CG	2.64	0.40
3:E:130:GLN:NE2	3:E:183:PHE:O	2.54	0.40
3:E:151:TRP:CE2	3:E:214:LYS:HB3	2.56	0.40
3:E:320:ILE:CD1	3:E:339:LEU:HA	2.50	0.40
3:E:321:GLU:OE2	3:E:363:THR:OG1	2.31	0.40
3:E:551:PRO:O	3:E:552:GLU:HB3	2.19	0.40
3:F:166:ILE:CG1	3:F:168:MET:HG2	2.45	0.40
3:F:328:GLU:O	3:F:329:GLU:C	2.64	0.40
3:F:465:LEU:HD21	3:F:561:ALA:HB2	2.03	0.40
3:F:524:ILE:HD11	3:F:558:LEU:HB2	2.03	0.40
1:A:478:ASN:CG	1:A:479:SER:N	2.79	0.40
3:E:138:ASN:O	3:E:200:GLU:CD	2.64	0.40
3:E:329:GLU:HG2	3:E:380:LEU:HD11	2.02	0.40
3:E:453:VAL:HG23	3:E:454:LEU:CD2	2.51	0.40
3:F:331:VAL:H	3:F:331:VAL:HG23	1.59	0.40
3:F:444:PRO:HA	3:F:447:ILE:CG1	2.49	0.40
1:C:521:PHE:HD1	1:C:569:PHE:CG	2.39	0.40
3:E:27:GLY:O	3:E:30:GLN:HG3	2.22	0.40
3:F:160:PRO:O	3:F:161:TYR:C	2.64	0.40
1:A:523:LYS:HE2	1:A:526:THR:HG21	2.03	0.40
1:C:476:HIS:O	1:C:477:GLN:HG2	2.21	0.40
1:C:558:GLU:OE2	1:C:612:LEU:HD22	2.22	0.40
3:E:185:LYS:O	3:E:188:VAL:HG12	2.21	0.40
3:E:194:ASN:HD22	3:E:201:ASN:ND2	2.19	0.40
3:F:137:HIS:NE2	3:F:138:ASN:HB3	2.37	0.40
3:F:375:CYS:HA	3:F:376:PRO:HD3	1.75	0.40
1:C:555:LEU:HA	1:C:556:PRO:HD3	1.81	0.40
3:E:321:GLU:O	3:E:325:GLN:HG2	2.21	0.40
3:F:110:ILE:HG13	3:F:110:ILE:H	1.72	0.40
3:F:157:LEU:H	3:F:157:LEU:HG	1.75	0.40
3:F:295:VAL:HG11	3:F:337:GLU:OE1	2.21	0.40
3:F:318:GLY:O	3:F:321:GLU:HB3	2.22	0.40
3:F:330:SER:OG	3:F:331:VAL:N	2.54	0.40
3:F:516:SER:HB2	3:F:565:PHE:CZ	2.57	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	252/282 (89%)	225 (89%)	26 (10%)	1 (0%)	30	65
1	C	246/282 (87%)	228 (93%)	17 (7%)	1 (0%)	30	65
2	B	80/106 (76%)	72 (90%)	8 (10%)	0	100	100
2	D	83/106 (78%)	76 (92%)	6 (7%)	1 (1%)	10	40
3	E	509/596 (85%)	464 (91%)	44 (9%)	1 (0%)	43	76
3	F	492/596 (83%)	450 (92%)	40 (8%)	2 (0%)	30	65
All	All	1662/1968 (84%)	1515 (91%)	141 (8%)	6 (0%)	30	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	530	PRO
3	E	306	VAL
2	D	65	SER
3	F	113	PRO
1	A	489	ILE
3	F	48	ILE

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	237/258 (92%)	195 (82%)	42 (18%)	2	10
1	C	234/258 (91%)	191 (82%)	43 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	74/90 (82%)	55 (74%)	19 (26%)	0	3
2	D	75/90 (83%)	59 (79%)	16 (21%)	1	6
3	E	481/548 (88%)	386 (80%)	95 (20%)	1	8
3	F	471/548 (86%)	382 (81%)	89 (19%)	1	9
All	All	1572/1792 (88%)	1268 (81%)	304 (19%)	1	8

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	LEU
1	A	427	ASP
1	A	429	LEU
1	A	430	LEU
1	A	445	THR
1	A	446	LEU
1	A	454	LYS
1	A	459	LYS
1	A	461	VAL
1	A	463	GLN
1	A	474	LEU
1	A	482	ASP
1	A	483	ASP
1	A	490	SER
1	A	499	GLU
1	A	504	LEU
1	A	511	ILE
1	A	523	LYS
1	A	526	THR
1	A	527	ASN
1	A	532	ASP
1	A	534	ASP
1	A	536	SER
1	A	538	GLN
1	A	544	SER
1	A	552	THR
1	A	559	LEU
1	A	567	THR
1	A	591	VAL
1	A	598	ARG
1	A	617	GLU
1	A	618	ASP

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Mol	Chain	Res	Type
1	A	621	THR
1	A	633	MET
1	A	641	GLN
1	A	645	LYS
1	A	646	SER
1	A	648	LEU
1	A	679	LYS
1	A	686	VAL
1	A	688	MET
1	A	689	LYS
2	B	20	LYS
2	B	23	GLU
2	B	30	VAL
2	B	38	VAL
2	B	39	VAL
2	B	49	ILE
2	B	53	CYS
2	B	60	GLN
2	B	62	SER
2	B	64	THR
2	B	74	VAL
2	B	77	HIS
2	B	82	HIS
2	B	86	ARG
2	B	89	LYS
2	B	91	ARG
2	B	93	VAL
2	B	96	LEU
2	B	104	GLN
1	C	431	LYS
1	C	442	LEU
1	C	443	GLU
1	C	447	ASN
1	C	448	GLN
1	C	450	MET
1	C	461	VAL
1	C	481	SER
1	C	483	ASP
1	C	489	ILE
1	C	494	GLN
1	C	501	THR
1	C	513	VAL

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Mol	Chain	Res	Type
1	C	518	ASN
1	C	524	HIS
1	C	525	LEU
1	C	526	THR
1	C	533	LEU
1	C	534	ASP
1	C	538	GLN
1	C	539	VAL
1	C	549	GLN
1	C	552	THR
1	C	562	SER
1	C	564	GLN
1	C	572	SER
1	C	577	ARG
1	C	596	LYS
1	C	617	GLU
1	C	618	ASP
1	C	621	THR
1	C	626	THR
1	C	633	MET
1	C	634	ASP
1	C	642	ILE
1	C	654	GLU
1	C	658	VAL
1	C	661	VAL
1	C	662	GLU
1	C	666	ASP
1	C	668	LEU
1	C	682	VAL
1	C	688	MET
2	D	20	LYS
2	D	24	VAL
2	D	28	ASN
2	D	37	ILE
2	D	49	ILE
2	D	50	MET
2	D	52	LEU
2	D	62	SER
2	D	68	CYS
2	D	69	THR
2	D	74	VAL
2	D	86	ARG

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Mol	Chain	Res	Type
2	D	87	TRP
2	D	92	GLN
2	D	93	VAL
2	D	102	GLU
3	E	1	MET
3	E	3	VAL
3	E	4	GLU
3	E	6	LEU
3	E	8	SER
3	E	31	LEU
3	E	41	HIS
3	E	42	THR
3	E	43	ASP
3	E	44	GLN
3	E	49	ILE
3	E	53	LYS
3	E	54	ASN
3	E	56	VAL
3	E	77	ASP
3	E	79	GLU
3	E	92	LEU
3	E	94	VAL
3	E	102	LEU
3	E	103	LEU
3	E	108	GLU
3	E	116	LYS
3	E	118	ILE
3	E	119	SER
3	E	127	GLN
3	E	130	GLN
3	E	131	THR
3	E	133	ILE
3	E	145	LEU
3	E	149	THR
3	E	154	LEU
3	E	155	SER
3	E	156	LEU
3	E	163	LYS
3	E	170	ASP
3	E	184	THR
3	E	189	GLU
3	E	190	GLU

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Mol	Chain	Res	Type
3	E	193	ASP
3	E	208	LEU
3	E	209	LEU
3	E	216	LEU
3	E	222	THR
3	E	253	HIS
3	E	258	MET
3	E	281	GLN
3	E	293	VAL
3	E	305	MET
3	E	306	VAL
3	E	307	LEU
3	E	312	LEU
3	E	326	ARG
3	E	338	LEU
3	E	344	LEU
3	E	354	GLN
3	E	358	ILE
3	E	359	LYS
3	E	363	THR
3	E	371	VAL
3	E	375	CYS
3	E	377	ILE
3	E	398	GLN
3	E	414	SER
3	E	416	VAL
3	E	421	ILE
3	E	432	LEU
3	E	439	LYS
3	E	440	TRP
3	E	442	THR
3	E	450	LEU
3	E	455	PHE
3	E	458	GLU
3	E	461	GLU
3	E	462	THR
3	E	465	LEU
3	E	466	GLN
3	E	486	ASN
3	E	490	ASN
3	E	492	THR
3	E	494	LEU

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Mol	Chain	Res	Type
3	E	496	THR
3	E	498	LEU
3	E	500	ASN
3	E	517	LYS
3	E	531	GLN
3	E	535	ASP
3	E	552	GLU
3	E	555	LEU
3	E	556	LYS
3	E	557	VAL
3	E	576	GLU
3	E	579	ILE
3	E	581	ILE
3	E	582	LYS
3	E	583	THR
3	F	3	VAL
3	F	8	SER
3	F	18	GLU
3	F	19	GLN
3	F	25	ASP
3	F	31	LEU
3	F	38	GLU
3	F	45	LEU
3	F	46	LEU
3	F	47	GLU
3	F	49	ILE
3	F	58	ILE
3	F	59	LYS
3	F	61	MET
3	F	85	VAL
3	F	96	LEU
3	F	97	CYS
3	F	103	LEU
3	F	107	LEU
3	F	108	GLU
3	F	112	GLU
3	F	116	LYS
3	F	123	LEU
3	F	124	LEU
3	F	125	LEU
3	F	131	THR
3	F	132	VAL

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Mol	Chain	Res	Type
3	F	139	LYS
3	F	166	ILE
3	F	167	GLN
3	F	174	CYS
3	F	180	LEU
3	F	181	ILE
3	F	185	LYS
3	F	188	VAL
3	F	190	GLU
3	F	191	VAL
3	F	192	ILE
3	F	201	ASN
3	F	215	SER
3	F	238	ARG
3	F	248	LEU
3	F	249	SER
3	F	251	ILE
3	F	279	ASN
3	F	280	LYS
3	F	296	GLN
3	F	300	ILE
3	F	302	GLN
3	F	326	ARG
3	F	330	SER
3	F	331	VAL
3	F	332	ILE
3	F	348	ASP
3	F	354	GLN
3	F	356	LEU
3	F	357	GLU
3	F	362	LEU
3	F	377	ILE
3	F	379	THR
3	F	396	ASP
3	F	402	THR
3	F	410	THR
3	F	442	THR
3	F	448	SER
3	F	450	LEU
3	F	452	LEU
3	F	454	LEU
3	F	465	LEU

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Mol	Chain	Res	Type
3	F	466	GLN
3	F	478	LEU
3	F	479	ARG
3	F	488	ASN
3	F	491	GLN
3	F	494	LEU
3	F	496	THR
3	F	509	LEU
3	F	510	HIS
3	F	514	ASN
3	F	516	SER
3	F	524	ILE
3	F	531	GLN
3	F	532	LYS
3	F	554	GLN
3	F	560	SER
3	F	562	LEU
3	F	581	ILE
3	F	582	LYS
3	F	583	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	ASN
1	A	520	GLN
1	A	524	HIS
1	A	548	GLN
1	A	597	ASN
1	A	630	GLN
1	A	641	GLN
1	A	677	ASN
1	A	683	ASN
1	A	685	ASN
2	B	28	ASN
2	B	77	HIS
1	C	478	ASN
1	C	518	ASN
1	C	527	ASN
1	C	602	GLN
1	C	623	GLN
1	C	638	GLN

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Mol	Chain	Res	Type
2	D	60	GLN
3	E	30	GLN
3	E	41	HIS
3	E	152	ASN
3	E	153	GLN
3	E	194	ASN
3	E	253	HIS
3	E	296	GLN
3	E	319	HIS
3	E	325	GLN
3	E	413	HIS
3	E	422	GLN
3	E	445	GLN
3	E	467	ASN
3	E	504	ASN
3	F	7	GLN
3	F	14	GLN
3	F	34	GLN
3	F	50	GLN
3	F	60	ASN
3	F	98	ASN
3	F	120	GLN
3	F	153	GLN
3	F	201	ASN
3	F	224	GLN
3	F	279	ASN
3	F	296	GLN
3	F	302	GLN
3	F	319	HIS
3	F	341	ASN
3	F	366	GLN
3	F	398	GLN
3	F	409	ASN
3	F	422	GLN
3	F	423	ASN
3	F	466	GLN
3	F	486	ASN
3	F	488	ASN

5.3.3 RNA ⓘ

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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	258/282 (91%)	-0.05	7 (2%)	56 33	51, 88, 168, 204	0
1	C	254/282 (90%)	0.12	10 (3%)	43 24	60, 99, 174, 207	0
2	B	84/106 (79%)	0.14	1 (1%)	76 55	52, 114, 156, 217	0
2	D	85/106 (80%)	0.00	1 (1%)	76 55	69, 100, 152, 169	0
3	E	523/596 (87%)	0.01	10 (1%)	66 43	49, 99, 165, 213	0
3	F	512/596 (85%)	0.09	15 (2%)	53 31	54, 119, 170, 212	0
All	All	1716/1968 (87%)	0.05	44 (2%)	57 34	49, 104, 169, 217	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	451	GLU	5.0
1	A	442	LEU	4.6
3	F	46	LEU	4.3
1	C	421	GLU	4.1
1	A	451	GLU	4.0
1	A	421	GLU	3.8
3	E	13	CYS	3.7
2	B	22	PHE	3.6
3	E	54	ASN	3.5
1	A	647	LYS	3.5
3	F	439	LYS	3.3
3	F	61	MET	3.2
1	C	455	LYS	3.1
1	C	497	GLY	3.0
3	E	467	ASN	3.0
1	C	531	LEU	3.0
1	A	455	LYS	2.9
3	F	49	ILE	2.9
3	F	57	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
3	E	550	PRO	2.8
1	A	422	LEU	2.8
3	F	45	LEU	2.8
1	A	452	LYS	2.7
1	C	452	LYS	2.7
1	C	419	PRO	2.7
3	E	110	ILE	2.7
1	C	456	ILE	2.6
3	F	550	PRO	2.6
3	F	224	GLN	2.5
3	E	42	THR	2.5
3	E	1	MET	2.5
3	E	226	PHE	2.4
3	E	4	GLU	2.3
3	F	171	TYR	2.3
3	E	495	TRP	2.3
3	F	18	GLU	2.2
1	C	442	LEU	2.2
1	C	576	GLY	2.2
3	F	161	TYR	2.2
3	F	461	GLU	2.1
3	F	462	THR	2.1
2	D	50	MET	2.1
3	F	115	GLY	2.0
3	F	60	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
4	ZN	B	201	1/1	0.99	0.06	91,91,91,91	0
4	ZN	B	203	1/1	0.99	0.04	112,112,112,112	0
4	ZN	D	202	1/1	0.99	0.03	120,120,120,120	0
4	ZN	D	203	1/1	0.99	0.04	101,101,101,101	0
4	ZN	B	202	1/1	1.00	0.02	96,96,96,96	0
4	ZN	D	201	1/1	1.00	0.02	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.