



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:32 AM UTC

PDB ID : 3TKN / pdb_00003tkn
Title : Structure of the Nup82-Nup159-Nup98 heterotrimer
Authors : Stuwe, T.T.; Hoelz, A.
Deposited on : 2011-08-28
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

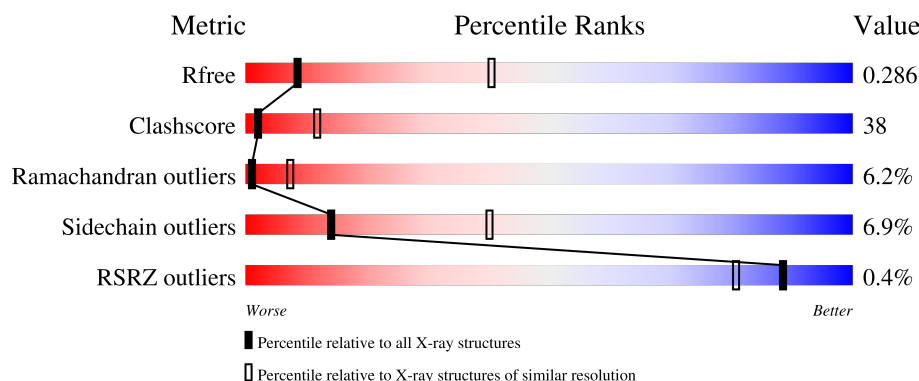
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	452	39% 50% 11%
1	D	452	40% 49% 10% .
1	G	452	36% 52% 11% .
2	B	39	46% 21% 5% 28%
2	E	39	33% 33% 5% 28%

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Mol	Chain	Length	Quality of chain
2	H	39	38%28%. .28%
3	C	152	36%51%9% . .
3	F	152	% 38%49%9% . .
3	I	152	% 37%51%8% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15021 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 Nucleoporin NUP82.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3628	2323	587	707	11			
1	D	447	Total	C	N	O	S	0	0	0
			3601	2309	582	699	11			
1	G	447	Total	C	N	O	S	0	0	0
			3601	2309	582	699	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	SER	CYS	conflict	UNP P40368
D	396	SER	CYS	conflict	UNP P40368
G	396	SER	CYS	conflict	UNP P40368

- Molecule 2 is a protein called Nucleoporin NUP159.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	28	Total	C	N	O	S	0	0	0
			221	144	37	37	3			
2	E	28	Total	C	N	O	S	0	0	0
			221	144	37	37	3			
2	H	28	Total	C	N	O	S	0	0	0
			221	144	37	37	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1422	GLY	-	expression tag	UNP P40477
B	1423	PRO	-	expression tag	UNP P40477
B	1424	HIS	-	expression tag	UNP P40477
E	1422	GLY	-	expression tag	UNP P40477
E	1423	PRO	-	expression tag	UNP P40477

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1424	HIS	-	expression tag	UNP P40477
H	1422	GLY	-	expression tag	UNP P40477
H	1423	PRO	-	expression tag	UNP P40477
H	1424	HIS	-	expression tag	UNP P40477

- Molecule 3 is a protein called Nucleoporin 98.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	147	Total	C	N	O	S	0	0	0
			1176	745	202	226	3			
3	F	147	Total	C	N	O	S	0	0	0
			1176	745	202	226	3			
3	I	147	Total	C	N	O	S	0	0	0
			1176	745	202	226	3			

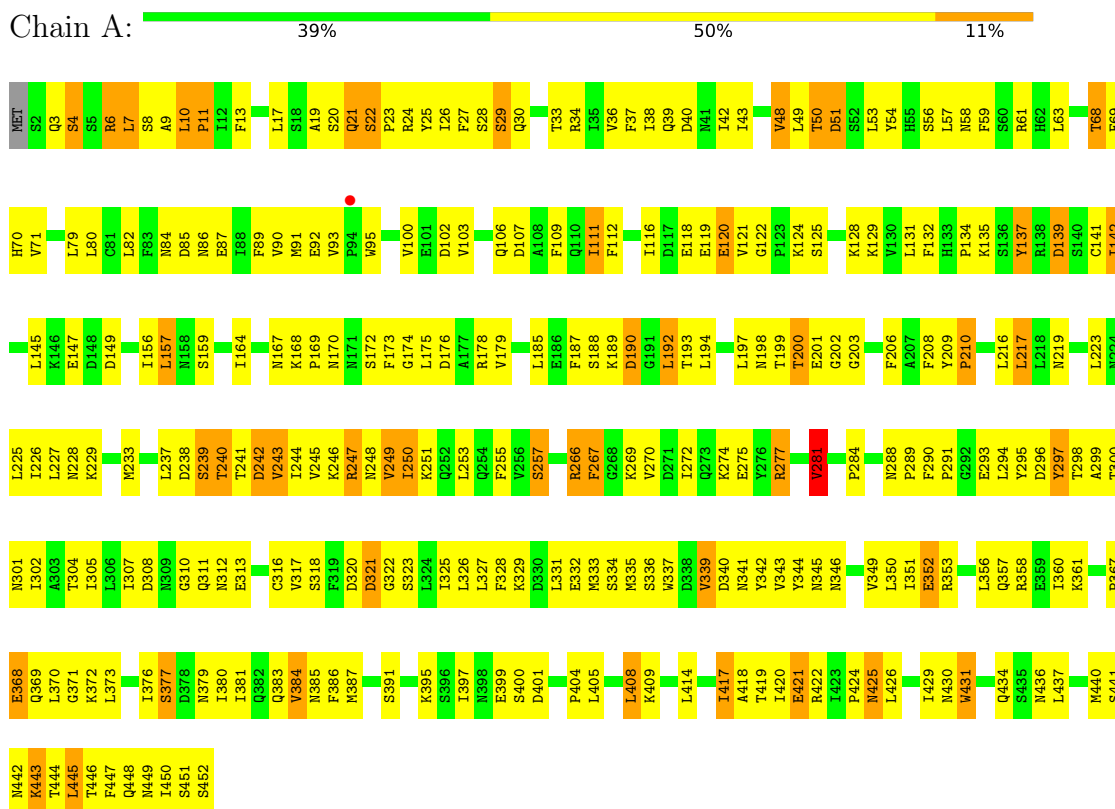
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	729	GLY	-	expression tag	UNP Q6PFD9
C	730	PRO	-	expression tag	UNP Q6PFD9
C	731	HIS	-	expression tag	UNP Q6PFD9
F	729	GLY	-	expression tag	UNP Q6PFD9
F	730	PRO	-	expression tag	UNP Q6PFD9
F	731	HIS	-	expression tag	UNP Q6PFD9
I	729	GLY	-	expression tag	UNP Q6PFD9
I	730	PRO	-	expression tag	UNP Q6PFD9
I	731	HIS	-	expression tag	UNP Q6PFD9

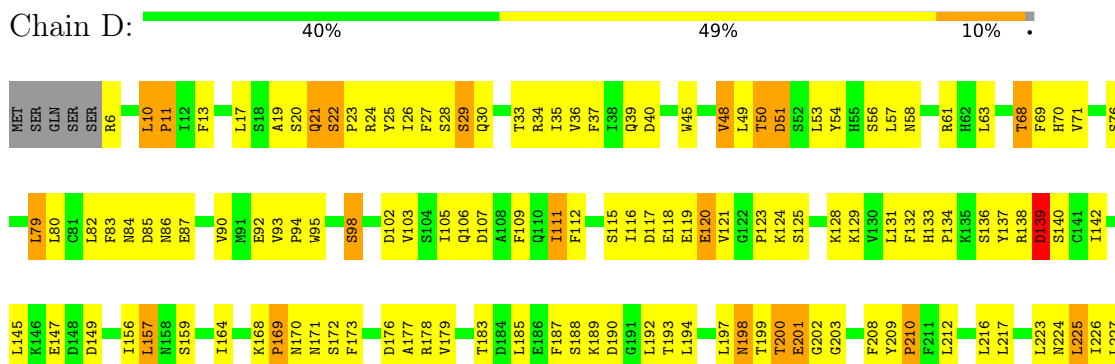
3 Residue-property plots

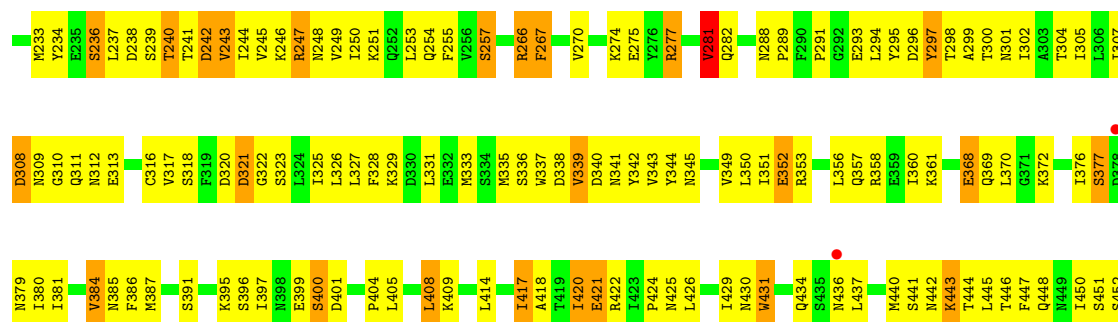
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nucleoporin NUP82



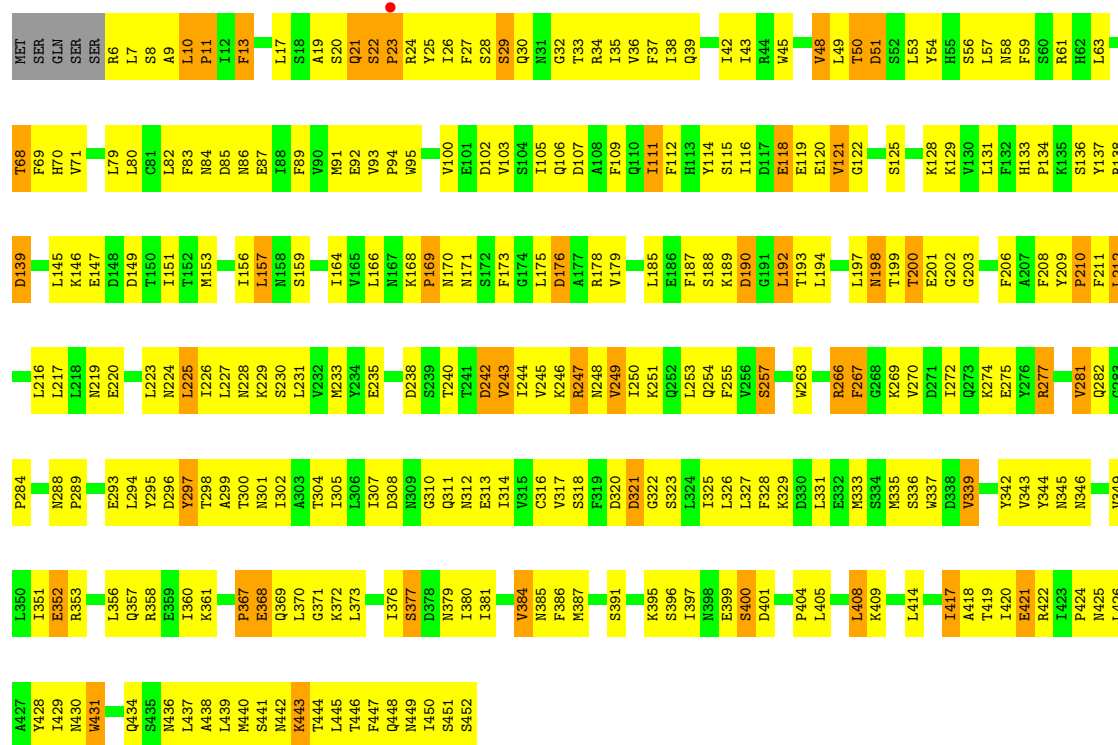
• Molecule 1: Nucleoporin NUP82





• Molecule 1: Nucleoporin NUP82

Chain G: 36% 52% 11%



• Molecule 2: Nucleoporin NUP159

Chain B: 46% 21% 5% 28%

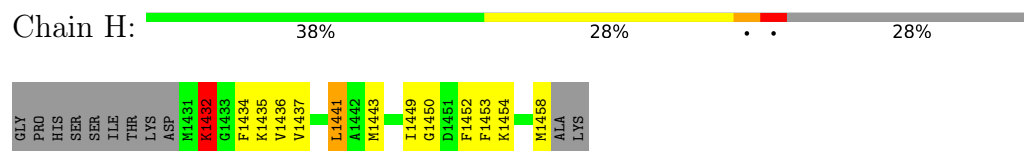


• Molecule 2: Nucleoporin NUP159

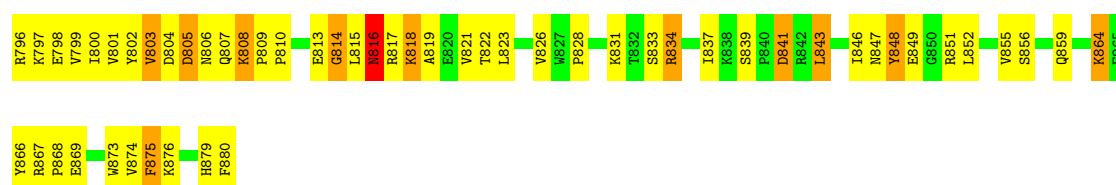
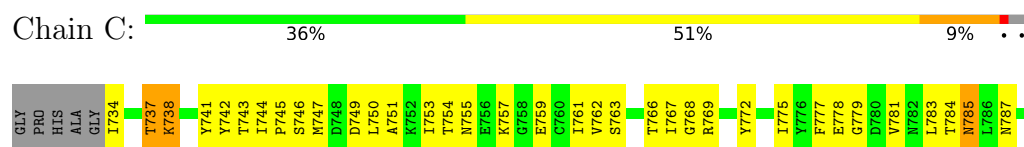
Chain E: 33% 33% 5% 28%



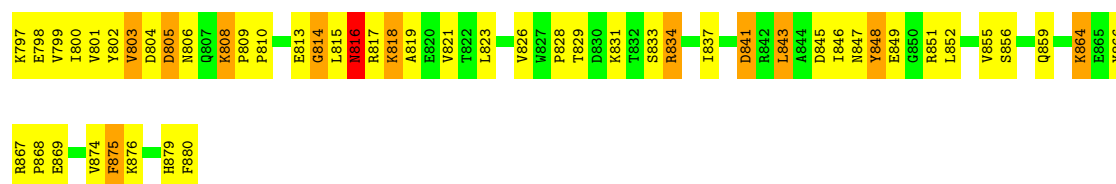
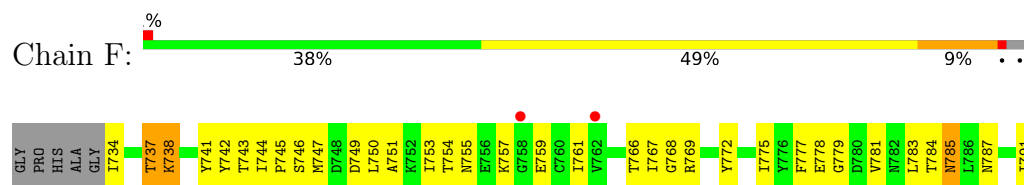
- Molecule 2: Nucleoporin NUP159



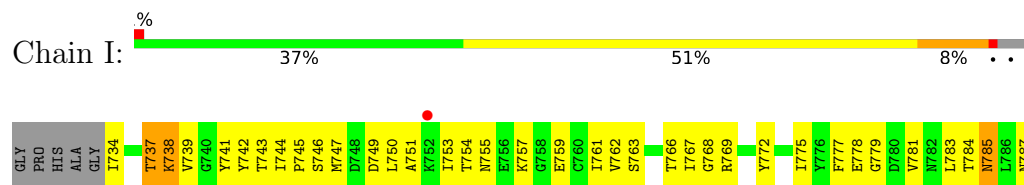
- Molecule 3: Nucleoporin 98



- Molecule 3: Nucleoporin 98



- Molecule 3: Nucleoporin 98



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.91Å 115.85Å 118.49Å 90.00° 111.06° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.40) 92.3 (20.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.285 0.250 , 0.286	Depositor DCC
R_{free} test set	3659 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	96.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15021	wwPDB-VP
Average B, all atoms (Å ²)	113.0	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

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	0.55	0/3701	1.03	17/5025 (0.3%)
1	D	0.65	0/3674	1.02	16/4989 (0.3%)
1	G	0.53	0/3674	1.03	14/4989 (0.3%)
2	B	0.73	0/223	0.98	0/293
2	E	0.84	0/223	0.98	1/293 (0.3%)
2	H	0.69	0/223	0.98	1/293 (0.3%)
3	C	0.42	0/1199	0.93	5/1620 (0.3%)
3	F	0.47	0/1199	0.93	5/1620 (0.3%)
3	I	0.41	0/1199	0.91	5/1620 (0.3%)
All	All	0.56	0/15315	1.00	64/20742 (0.3%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	239	SER	N-CA-C	-8.12	105.37	114.62
1	D	111	ILE	N-CA-C	8.11	118.89	110.62
1	G	190	ASP	N-CA-C	-7.96	103.58	113.38
1	G	111	ILE	N-CA-C	7.70	118.48	110.62
1	D	190	ASP	N-CA-C	-7.59	104.04	113.38
1	A	111	ILE	N-CA-C	7.50	118.27	110.62
1	A	190	ASP	N-CA-C	-7.14	104.59	113.38
1	G	68	THR	N-CA-C	-6.60	105.14	113.72
1	A	68	THR	N-CA-C	-6.59	105.15	113.72
1	G	400	SER	N-CA-C	-6.53	102.92	111.74
1	A	317	VAL	N-CA-C	6.46	117.16	108.11
1	A	400	SER	N-CA-C	-6.44	103.04	111.74
1	D	68	THR	N-CA-C	-6.36	105.45	113.72
1	D	400	SER	N-CA-C	-6.35	103.16	111.74
3	F	848	TYR	N-CA-C	-6.29	104.52	111.82
1	D	56	SER	N-CA-C	6.25	116.53	108.34
1	D	317	VAL	N-CA-C	6.25	116.86	108.11
1	G	317	VAL	N-CA-C	6.17	116.75	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	867	ARG	CA-C-N	6.12	125.60	119.24
3	F	867	ARG	C-N-CA	6.12	125.60	119.24
3	I	848	TYR	N-CA-C	-6.10	104.74	111.82
3	F	856	SER	N-CA-C	-6.08	104.21	111.69
3	C	867	ARG	CA-C-N	5.98	125.46	119.24
3	C	867	ARG	C-N-CA	5.98	125.46	119.24
3	C	856	SER	N-CA-C	-5.98	104.34	111.69
3	C	848	TYR	N-CA-C	-5.96	104.90	111.82
1	G	192	LEU	N-CA-C	-5.94	107.26	114.75
1	A	250	ILE	N-CA-C	-5.88	105.00	110.53
3	I	867	ARG	CA-C-N	5.84	125.31	119.24
3	I	867	ARG	C-N-CA	5.84	125.31	119.24
1	G	56	SER	N-CA-C	5.77	115.90	108.34
1	A	281	VAL	N-CA-C	5.71	116.94	109.58
3	I	739	VAL	N-CA-C	5.71	116.78	109.30
3	C	805	ASP	N-CA-C	-5.67	105.27	113.21
1	G	243	VAL	N-CA-C	5.66	116.30	110.36
1	A	192	LEU	N-CA-C	-5.64	107.65	114.75
1	D	177	ALA	N-CA-C	5.62	117.41	111.28
1	A	56	SER	N-CA-C	5.61	115.69	108.34
1	A	70	HIS	N-CA-C	-5.59	99.91	109.24
1	G	70	HIS	N-CA-C	-5.57	99.94	109.24
1	D	243	VAL	N-CA-C	5.55	116.19	110.36
1	A	240	THR	N-CA-C	-5.54	105.78	112.54
1	D	192	LEU	N-CA-C	-5.54	107.77	114.75
3	I	856	SER	N-CA-C	-5.47	104.96	111.69
1	D	170	ASN	N-CA-C	5.46	122.43	110.80
1	A	243	VAL	N-CA-C	5.43	116.07	110.36
3	F	805	ASP	N-CA-C	-5.43	105.61	113.21
1	D	339	VAL	N-CA-C	5.38	120.53	109.34
1	G	339	VAL	N-CA-C	5.38	120.53	109.34
1	D	70	HIS	N-CA-C	-5.37	100.27	109.24
2	H	1432	LYS	N-CA-C	5.34	115.44	108.07
1	A	132	PHE	N-CA-C	-5.32	101.03	109.76
1	A	339	VAL	N-CA-C	5.32	120.40	109.34
1	D	281	VAL	N-CA-C	5.30	116.42	109.58
1	D	212	LEU	N-CA-C	5.26	118.49	110.50
1	D	132	PHE	N-CA-C	-5.19	101.25	109.76
1	A	425	ASN	N-CA-C	-5.17	101.68	109.85
1	D	79	LEU	N-CA-C	5.11	117.44	109.52
1	G	169	PRO	N-CA-C	-5.10	101.96	112.47
1	G	212	LEU	N-CA-C	5.09	118.24	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	118	GLU	N-CA-C	-5.08	107.76	114.31
1	A	334	SER	N-CA-C	-5.07	101.60	109.72
1	G	13	PHE	N-CA-C	5.07	119.46	113.28
2	E	1448	GLN	N-CA-C	-5.06	105.84	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	0	3594	275	0
1	D	3601	0	3571	263	0
1	G	3601	0	3571	291	0
2	B	221	0	235	13	0
2	E	221	0	235	18	0
2	H	221	0	235	17	0
3	C	1176	0	1170	112	0
3	F	1176	0	1170	108	0
3	I	1176	0	1170	104	0
All	All	15021	0	14951	1135	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 38.

All (1135) 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:G:37:PHE:HE1	1:G:440:MET:HE1	1.15	1.10
1:G:57:LEU:HD22	1:G:100:VAL:HG11	1.36	1.02
1:A:121:VAL:HG12	1:A:122:GLY:H	1.32	0.95
1:A:6:ARG:HB2	1:A:431:TRP:HH2	1.30	0.93
1:D:142:ILE:HG23	1:D:156:ILE:HD11	1.53	0.89
1:D:381:ILE:HD11	1:D:424:PRO:HG3	1.55	0.89
1:A:381:ILE:HD11	1:A:424:PRO:HG3	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:PHE:CE1	1:G:440:MET:HE1	2.07	0.88
1:G:381:ILE:HD11	1:G:424:PRO:HG3	1.54	0.87
1:G:112:PHE:HB2	1:G:156:ILE:HG23	1.55	0.87
1:A:384:VAL:HG13	1:A:414:LEU:HD13	1.56	0.86
1:D:169:PRO:HA	1:D:178:ARG:HH11	1.40	0.86
1:G:368:GLU:H	1:G:368:GLU:CD	1.84	0.85
1:D:384:VAL:HG13	1:D:414:LEU:HD13	1.60	0.84
1:A:6:ARG:HB2	1:A:431:TRP:CH2	2.13	0.84
1:G:384:VAL:HG13	1:G:414:LEU:HD13	1.58	0.84
1:G:169:PRO:HA	1:G:178:ARG:HH11	1.42	0.83
1:G:267:PHE:HD1	1:G:267:PHE:H	1.27	0.83
1:G:208:PHE:CZ	1:G:281:VAL:HG22	2.12	0.82
2:B:1434:PHE:HD1	2:B:1435:LYS:H	1.26	0.82
1:D:267:PHE:H	1:D:267:PHE:HD1	1.26	0.82
2:E:1434:PHE:HD1	2:E:1435:LYS:H	1.26	0.82
1:D:203:GLY:O	3:F:831:LYS:HE3	1.80	0.82
1:A:368:GLU:CD	1:A:368:GLU:H	1.87	0.82
1:D:246:LYS:O	1:D:250:ILE:HG12	1.80	0.82
1:A:174:GLY:H	3:C:859:GLN:HE22	1.26	0.81
1:G:247:ARG:HH11	1:G:247:ARG:HG2	1.45	0.81
2:H:1434:PHE:HD1	2:H:1435:LYS:H	1.27	0.81
3:C:864:LYS:HE3	3:C:876:LYS:HE2	1.61	0.81
1:D:368:GLU:CD	1:D:368:GLU:H	1.89	0.81
3:I:864:LYS:HE3	3:I:876:LYS:HE2	1.63	0.80
1:G:210:PRO:HG3	1:G:335:MET:HE3	1.61	0.80
1:G:255:PHE:CD2	1:G:335:MET:HE1	2.17	0.80
1:G:179:VAL:HG21	1:G:281:VAL:HG11	1.63	0.79
1:D:169:PRO:HA	1:D:178:ARG:NH1	1.98	0.79
1:G:246:LYS:O	1:G:250:ILE:HG12	1.81	0.79
1:A:137:TYR:HH	1:A:267:PHE:HD2	1.31	0.79
1:A:6:ARG:CB	1:A:431:TRP:HH2	1.97	0.78
1:A:129:LYS:HE2	1:A:131:LEU:HD21	1.65	0.78
1:A:267:PHE:HD1	1:A:267:PHE:H	1.27	0.78
1:D:247:ARG:HG2	1:D:247:ARG:HH11	1.46	0.78
3:F:864:LYS:HE3	3:F:876:LYS:HE2	1.63	0.78
1:D:179:VAL:HG21	1:D:281:VAL:HG11	1.66	0.78
1:A:30:GLN:HG3	1:A:34:ARG:HD3	1.65	0.78
1:D:142:ILE:CG2	1:D:156:ILE:HD11	2.13	0.78
1:A:208:PHE:CZ	1:A:281:VAL:HG22	2.19	0.77
1:A:247:ARG:HG2	1:A:247:ARG:HH11	1.49	0.77
3:C:805:ASP:HA	3:C:808:LYS:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:LYS:HE2	1:G:131:LEU:HD21	1.66	0.77
1:A:125:SER:OG	1:A:147:GLU:HB2	1.84	0.77
1:A:301:ASN:H	1:A:318:SER:HB2	1.50	0.77
1:G:30:GLN:HG3	1:G:34:ARG:HD3	1.67	0.77
3:I:805:ASP:HA	3:I:808:LYS:HB2	1.67	0.77
3:F:805:ASP:HA	3:F:808:LYS:HB2	1.67	0.77
1:A:27:PHE:HZ	1:A:71:VAL:HG23	1.50	0.76
3:I:767:ILE:HD13	3:I:792:VAL:HG11	1.67	0.76
1:D:30:GLN:HG3	1:D:34:ARG:HD3	1.67	0.76
3:F:851:ARG:HH21	3:F:851:ARG:HG3	1.51	0.76
1:G:27:PHE:HZ	1:G:71:VAL:HG23	1.49	0.76
1:A:255:PHE:CD2	1:A:335:MET:HE1	2.20	0.75
1:D:210:PRO:HG3	1:D:335:MET:HE3	1.68	0.75
3:I:767:ILE:CD1	3:I:792:VAL:HG11	2.17	0.75
3:F:767:ILE:CD1	3:F:792:VAL:HG11	2.17	0.75
3:I:851:ARG:HH21	3:I:851:ARG:HG3	1.51	0.75
1:A:300:THR:HB	1:A:318:SER:HB2	1.69	0.74
1:D:129:LYS:HE2	1:D:131:LEU:HD21	1.69	0.74
1:D:380:ILE:HG22	1:D:381:ILE:N	2.02	0.74
3:C:851:ARG:HH21	3:C:851:ARG:HG3	1.51	0.74
1:A:34:ARG:HB3	1:A:95:TRP:CH2	2.23	0.74
1:A:173:PHE:HA	3:C:859:GLN:OE1	1.86	0.74
1:A:358:ARG:CZ	1:A:380:ILE:HD12	2.17	0.74
1:A:174:GLY:H	3:C:859:GLN:NE2	1.86	0.74
3:F:767:ILE:HD13	3:F:792:VAL:HG11	1.69	0.74
3:I:828:PRO:HG2	3:I:837:ILE:HB	1.69	0.74
1:A:425:ASN:C	1:A:426:LEU:HD12	2.13	0.73
1:D:238:ASP:CG	1:D:239:SER:H	1.96	0.73
2:E:1432:LYS:HD3	2:E:1432:LYS:C	2.12	0.73
1:G:405:LEU:HB3	2:H:1452:PHE:HE1	1.53	0.73
3:C:767:ILE:CD1	3:C:792:VAL:HG11	2.18	0.73
1:D:27:PHE:HZ	1:D:71:VAL:HG23	1.51	0.73
1:D:37:PHE:HE1	1:D:440:MET:HE1	1.52	0.73
1:A:349:VAL:HG11	2:B:1453:PHE:HB2	1.71	0.73
1:G:45:TRP:HH2	1:G:100:VAL:HG21	1.55	0.72
1:D:208:PHE:CZ	1:D:281:VAL:HG22	2.24	0.72
1:G:380:ILE:HG22	1:G:381:ILE:N	2.04	0.72
1:A:297:TYR:HB3	1:A:320:ASP:HB2	1.70	0.72
1:A:112:PHE:HB2	1:A:156:ILE:HG23	1.71	0.71
3:C:767:ILE:HD13	3:C:792:VAL:HG11	1.70	0.71
1:A:380:ILE:HG22	1:A:381:ILE:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:ARG:CZ	1:D:380:ILE:HD12	2.20	0.71
1:A:246:LYS:O	1:A:250:ILE:HG12	1.90	0.71
1:D:112:PHE:HB2	1:D:156:ILE:HG23	1.71	0.71
1:D:255:PHE:CD2	1:D:335:MET:HE1	2.25	0.71
1:A:174:GLY:N	3:C:859:GLN:HE22	1.89	0.71
3:C:828:PRO:HG2	3:C:837:ILE:HB	1.72	0.71
3:C:767:ILE:HG12	3:C:768:GLY:N	2.06	0.70
3:I:809:PRO:HG2	3:I:814:GLY:HA3	1.74	0.70
1:D:300:THR:HB	1:D:318:SER:HB2	1.73	0.70
1:A:210:PRO:HG3	1:A:335:MET:HE3	1.72	0.70
3:C:818:LYS:H	3:C:818:LYS:HD2	1.57	0.70
1:D:343:VAL:HG11	3:F:834:ARG:CZ	2.21	0.70
1:G:34:ARG:HB3	1:G:95:TRP:CH2	2.26	0.70
1:D:34:ARG:HB3	1:D:95:TRP:CH2	2.27	0.70
3:F:828:PRO:HG2	3:F:837:ILE:HB	1.73	0.70
3:F:767:ILE:HG12	3:F:768:GLY:N	2.05	0.70
1:G:169:PRO:HA	1:G:178:ARG:NH1	2.05	0.70
1:D:209:TYR:CE2	1:D:335:MET:HG3	2.27	0.69
1:D:425:ASN:C	1:D:426:LEU:HD12	2.17	0.69
1:A:443:LYS:H	1:A:443:LYS:HD2	1.58	0.69
1:G:37:PHE:HE1	1:G:440:MET:CE	2.00	0.69
1:G:326:LEU:HD12	1:G:352:GLU:HG2	1.74	0.69
1:G:358:ARG:CZ	1:G:380:ILE:HD12	2.21	0.69
1:G:301:ASN:H	1:G:318:SER:HB2	1.58	0.69
3:I:767:ILE:HG12	3:I:768:GLY:N	2.08	0.69
1:A:6:ARG:HD3	1:A:431:TRP:CH2	2.28	0.69
3:C:851:ARG:O	3:C:855:VAL:HG23	1.93	0.69
1:D:301:ASN:H	1:D:318:SER:HB2	1.57	0.69
1:G:238:ASP:OD2	1:G:240:THR:HG22	1.93	0.69
1:D:443:LYS:H	1:D:443:LYS:HD2	1.58	0.69
3:F:767:ILE:HG12	3:F:768:GLY:H	1.57	0.69
1:G:300:THR:HB	1:G:318:SER:HB2	1.74	0.69
1:G:425:ASN:C	1:G:426:LEU:HD12	2.18	0.69
3:I:818:LYS:H	3:I:818:LYS:HD2	1.58	0.68
3:C:833:SER:C	3:C:834:ARG:HG2	2.17	0.68
1:G:175:LEU:HD12	3:I:797:LYS:HB3	1.75	0.68
1:G:245:VAL:O	1:G:249:VAL:HG23	1.94	0.68
3:I:761:ILE:HG23	3:I:781:VAL:O	1.93	0.68
1:D:297:TYR:HB3	1:D:320:ASP:HB2	1.73	0.68
2:B:1458:MET:HE2	2:B:1458:MET:HA	1.76	0.68
1:D:441:SER:HB3	1:D:444:THR:HB	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:833:SER:C	3:F:834:ARG:HG2	2.18	0.68
1:G:441:SER:HB3	1:G:444:THR:HB	1.75	0.68
3:C:761:ILE:HG23	3:C:781:VAL:O	1.94	0.68
1:D:326:LEU:HD12	1:D:352:GLU:HG2	1.75	0.68
1:G:157:LEU:N	1:G:157:LEU:HD23	2.09	0.68
1:A:209:TYR:CE2	1:A:335:MET:HG3	2.28	0.67
1:A:441:SER:HB3	1:A:444:THR:HB	1.77	0.67
3:I:833:SER:C	3:I:834:ARG:HG2	2.18	0.67
1:G:247:ARG:HG2	1:G:247:ARG:NH1	2.09	0.67
3:C:809:PRO:HG2	3:C:814:GLY:HA3	1.77	0.67
1:D:245:VAL:O	1:D:249:VAL:HG23	1.95	0.67
1:G:210:PRO:CG	1:G:335:MET:HE3	2.24	0.67
1:G:267:PHE:CD1	1:G:267:PHE:N	2.63	0.67
2:H:1458:MET:HE2	2:H:1458:MET:HA	1.75	0.67
1:G:284:PRO:O	3:I:834:ARG:NH2	2.27	0.67
1:G:297:TYR:HB3	1:G:320:ASP:HB2	1.75	0.67
3:C:817:ARG:HH21	3:C:818:LYS:HD3	1.60	0.66
1:D:275:GLU:CD	1:D:275:GLU:H	2.03	0.66
1:D:349:VAL:HG11	2:E:1453:PHE:HB2	1.76	0.66
3:F:761:ILE:HG23	3:F:781:VAL:O	1.96	0.66
1:D:380:ILE:HG22	1:D:381:ILE:H	1.61	0.66
1:G:170:ASN:HD21	1:G:176:ASP:HB3	1.61	0.66
3:I:767:ILE:HG12	3:I:768:GLY:H	1.60	0.66
3:C:767:ILE:HG12	3:C:768:GLY:H	1.60	0.66
1:G:209:TYR:CE2	1:G:335:MET:HG3	2.31	0.66
1:G:443:LYS:H	1:G:443:LYS:HD2	1.60	0.66
1:A:322:GLY:HA2	1:A:360:ILE:HG13	1.78	0.66
1:A:426:LEU:HD23	1:A:437:LEU:HD11	1.77	0.66
1:A:3:GLN:O	1:A:3:GLN:HG2	1.96	0.66
3:F:851:ARG:O	3:F:855:VAL:HG23	1.95	0.66
1:G:179:VAL:CG2	1:G:281:VAL:HG11	2.26	0.66
1:G:275:GLU:CD	1:G:275:GLU:H	2.04	0.66
1:A:275:GLU:H	1:A:275:GLU:CD	2.03	0.65
1:A:321:ASP:OD2	1:A:323:SER:HB2	1.96	0.65
1:G:380:ILE:HG22	1:G:381:ILE:H	1.60	0.65
1:G:426:LEU:HD23	1:G:437:LEU:HD11	1.77	0.65
1:D:10:LEU:HG	1:D:11:PRO:HD2	1.76	0.65
1:G:10:LEU:HG	1:G:11:PRO:HD2	1.78	0.65
1:D:203:GLY:O	3:F:831:LYS:CE	2.44	0.65
1:D:426:LEU:HD23	1:D:437:LEU:HD11	1.78	0.65
1:D:200:THR:O	3:F:851:ARG:HD2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:ARG:HG2	1:D:247:ARG:NH1	2.09	0.65
1:D:297:TYR:CD1	1:D:297:TYR:N	2.63	0.65
1:G:121:VAL:HG12	1:G:122:GLY:H	1.61	0.65
1:G:216:LEU:HB3	1:G:270:VAL:CG1	2.27	0.65
1:G:297:TYR:N	1:G:297:TYR:CD1	2.64	0.65
1:A:10:LEU:HG	1:A:11:PRO:HD2	1.77	0.65
1:A:121:VAL:HG12	1:A:122:GLY:N	2.09	0.65
3:F:809:PRO:HG2	3:F:814:GLY:HA3	1.77	0.65
1:G:25:TYR:HD2	1:G:425:ASN:HD22	1.43	0.65
3:I:817:ARG:HH21	3:I:818:LYS:HD3	1.62	0.65
1:D:210:PRO:CG	1:D:335:MET:HE3	2.27	0.65
1:G:133:HIS:HB3	1:G:136:SER:HB3	1.79	0.65
1:G:349:VAL:HG11	2:H:1453:PHE:HB2	1.79	0.65
1:A:169:PRO:HA	1:A:178:ARG:HH11	1.61	0.64
1:A:326:LEU:HD12	1:A:352:GLU:HG2	1.79	0.64
1:D:267:PHE:CD1	1:D:267:PHE:N	2.63	0.64
1:A:174:GLY:HA2	3:C:873:TRP:CH2	2.33	0.64
1:A:157:LEU:HD23	1:A:157:LEU:N	2.12	0.64
2:E:1434:PHE:HD1	2:E:1435:LYS:N	1.96	0.64
1:A:267:PHE:N	1:A:267:PHE:CD1	2.66	0.64
3:F:817:ARG:HH21	3:F:818:LYS:HD3	1.61	0.64
3:F:818:LYS:H	3:F:818:LYS:HD2	1.60	0.64
1:A:198:ASN:O	1:A:203:GLY:HA2	1.98	0.64
3:F:746:SER:O	3:F:750:LEU:HG	1.97	0.64
1:A:245:VAL:O	1:A:249:VAL:HG23	1.98	0.64
3:I:851:ARG:O	3:I:855:VAL:HG23	1.96	0.64
1:A:297:TYR:CD1	1:A:297:TYR:N	2.64	0.63
1:D:157:LEU:N	1:D:157:LEU:HD23	2.13	0.63
1:G:208:PHE:CE1	1:G:281:VAL:HG22	2.33	0.63
1:A:119:GLU:O	1:A:124:LYS:HE2	1.97	0.63
1:A:179:VAL:HG21	1:A:281:VAL:HG11	1.79	0.63
3:C:746:SER:O	3:C:750:LEU:HG	1.98	0.63
1:A:302:ILE:HA	1:A:316:CYS:O	1.97	0.63
1:G:255:PHE:HD2	1:G:335:MET:HE1	1.64	0.63
1:A:300:THR:HB	1:A:318:SER:CB	2.29	0.63
1:G:322:GLY:HA2	1:G:360:ILE:HG13	1.81	0.63
1:A:197:LEU:HD21	1:A:299:ALA:HB1	1.81	0.63
2:H:1434:PHE:HD1	2:H:1435:LYS:N	1.96	0.63
1:G:267:PHE:HD1	1:G:267:PHE:N	1.95	0.63
1:G:302:ILE:HA	1:G:316:CYS:O	1.98	0.62
1:A:321:ASP:CG	1:A:323:SER:HB2	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ILE:HG22	1:A:381:ILE:H	1.63	0.62
1:G:7:LEU:HD22	1:G:436:ASN:ND2	2.15	0.62
1:A:57:LEU:HD22	1:A:100:VAL:HG11	1.82	0.62
1:A:79:LEU:HD23	1:A:92:GLU:HA	1.81	0.62
1:G:17:LEU:HD13	1:G:17:LEU:O	2.00	0.62
3:I:746:SER:O	3:I:750:LEU:HG	2.00	0.62
1:D:233:MET:HE2	1:D:233:MET:HA	1.82	0.62
1:D:321:ASP:OD2	1:D:323:SER:HB2	2.00	0.61
1:G:79:LEU:HD23	1:G:92:GLU:HA	1.82	0.61
1:D:17:LEU:HD13	1:D:17:LEU:O	1.99	0.61
1:A:405:LEU:HB3	2:B:1452:PHE:HE1	1.66	0.61
1:D:322:GLY:HA2	1:D:360:ILE:HG13	1.81	0.61
1:D:239:SER:OG	1:D:240:THR:N	2.34	0.61
1:A:63:LEU:HD11	1:A:69:PHE:CE2	2.36	0.61
1:D:198:ASN:O	1:D:203:GLY:HA2	2.01	0.61
1:G:198:ASN:O	1:G:203:GLY:HA2	2.01	0.61
1:A:331:LEU:HB3	1:A:345:ASN:OD1	2.01	0.61
1:A:19:ALA:C	1:A:21:GLN:H	2.09	0.61
1:A:253:LEU:O	1:A:257:SER:HB2	2.01	0.61
1:G:210:PRO:HD3	1:G:335:MET:HG2	1.82	0.61
3:F:808:LYS:HE3	3:F:880:PHE:O	2.01	0.61
1:G:19:ALA:C	1:G:21:GLN:H	2.09	0.61
1:G:331:LEU:HB3	1:G:345:ASN:OD1	2.00	0.61
2:B:1434:PHE:HD1	2:B:1435:LYS:N	1.97	0.60
1:G:297:TYR:CE2	1:G:321:ASP:HB3	2.36	0.60
1:A:17:LEU:HD13	1:A:17:LEU:O	2.01	0.60
1:D:179:VAL:HG23	1:D:281:VAL:HG21	1.81	0.60
1:A:107:ASP:C	1:A:109:PHE:H	2.10	0.60
1:A:189:LYS:N	1:A:313:GLU:OE1	2.33	0.60
1:D:63:LEU:HD11	1:D:69:PHE:CE2	2.36	0.60
1:G:321:ASP:OD2	1:G:323:SER:HB2	2.01	0.60
1:A:28:SER:O	1:A:29:SER:HB2	2.01	0.60
1:A:237:LEU:CD2	1:A:241:THR:HG21	2.31	0.60
1:D:321:ASP:CG	1:D:323:SER:HB2	2.26	0.60
1:D:250:ILE:HG21	2:H:1441:LEU:HG	1.83	0.60
1:D:19:ALA:C	1:D:21:GLN:H	2.09	0.60
1:D:137:TYR:CE2	1:D:138:ARG:HG3	2.36	0.60
1:G:115:SER:N	1:G:118:GLU:OE2	2.33	0.60
1:A:226:ILE:HG23	1:A:227:LEU:N	2.17	0.60
1:D:179:VAL:CG2	1:D:281:VAL:HG11	2.31	0.60
1:D:302:ILE:HA	1:D:316:CYS:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:808:LYS:HE3	3:I:880:PHE:O	2.02	0.59
1:G:321:ASP:CG	1:G:323:SER:HB2	2.28	0.59
2:E:1458:MET:HE2	2:E:1458:MET:HA	1.83	0.59
1:A:169:PRO:HA	1:A:178:ARG:NH1	2.18	0.59
1:G:253:LEU:O	1:G:257:SER:HB2	2.02	0.59
1:A:79:LEU:HD12	1:A:139:ASP:HB2	1.85	0.59
1:G:107:ASP:C	1:G:109:PHE:H	2.11	0.59
1:G:231:LEU:O	1:G:235:GLU:HG3	2.01	0.59
1:A:3:GLN:O	1:A:4:SER:C	2.44	0.59
1:G:57:LEU:HD13	1:G:100:VAL:HB	1.84	0.59
3:C:808:LYS:HE3	3:C:880:PHE:O	2.02	0.59
1:D:53:LEU:HD13	1:D:54:TYR:N	2.18	0.59
1:G:431:TRP:O	1:G:434:GLN:HB2	2.03	0.59
1:D:320:ASP:C	1:D:322:GLY:H	2.10	0.58
3:F:837:ILE:HG22	3:F:843:LEU:HD13	1.85	0.58
1:G:63:LEU:HD11	1:G:69:PHE:CE2	2.38	0.58
1:G:179:VAL:HG23	1:G:281:VAL:HG21	1.84	0.58
1:G:430:ASN:HA	1:G:434:GLN:O	2.03	0.58
1:A:208:PHE:CE1	1:A:281:VAL:HG22	2.37	0.58
3:C:769:ARG:NH1	3:C:772:TYR:HE1	2.00	0.58
1:G:28:SER:O	1:G:29:SER:HB2	2.02	0.58
1:A:305:ILE:HD12	1:A:305:ILE:N	2.19	0.58
1:D:79:LEU:HD23	1:D:92:GLU:HA	1.84	0.58
1:G:175:LEU:O	3:I:798:GLU:HB2	2.03	0.58
3:I:837:ILE:HG22	3:I:843:LEU:HD13	1.86	0.58
3:I:769:ARG:NH1	3:I:772:TYR:HE1	2.02	0.58
1:D:107:ASP:C	1:D:109:PHE:H	2.11	0.58
2:E:1432:LYS:HG3	2:E:1433:GLY:N	2.19	0.58
1:G:300:THR:HB	1:G:318:SER:CB	2.34	0.58
1:G:329:LYS:HE2	1:G:333:MET:HG3	1.85	0.58
1:D:300:THR:HB	1:D:318:SER:CB	2.33	0.58
1:D:267:PHE:HD1	1:D:267:PHE:N	1.96	0.57
1:D:298:THR:HG22	1:D:299:ALA:N	2.19	0.57
3:F:851:ARG:HG3	3:F:851:ARG:NH2	2.19	0.57
1:G:29:SER:HB3	1:G:34:ARG:HB2	1.85	0.57
2:B:1441:LEU:HG	1:G:250:ILE:HG21	1.85	0.57
1:G:216:LEU:HB2	1:G:272:ILE:CD1	2.34	0.57
1:A:7:LEU:C	1:A:9:ALA:H	2.13	0.57
1:A:29:SER:HB3	1:A:34:ARG:HB2	1.87	0.57
1:A:37:PHE:HE1	1:A:440:MET:HE1	1.69	0.57
1:A:145:LEU:HD22	1:A:185:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PHE:HD1	1:A:267:PHE:N	1.98	0.57
1:G:125:SER:OG	1:G:147:GLU:HB2	2.04	0.57
2:E:1432:LYS:C	2:E:1432:LYS:CD	2.77	0.57
1:G:300:THR:HG22	1:G:301:ASN:OD1	2.05	0.57
1:G:405:LEU:HB3	2:H:1452:PHE:CE1	2.38	0.57
1:A:307:ILE:HG12	1:A:312:ASN:O	2.05	0.57
1:A:387:MET:HE3	1:A:391:SER:HB3	1.86	0.57
3:C:837:ILE:HG22	3:C:843:LEU:HD13	1.87	0.57
1:G:451:SER:O	1:G:452:SER:HB3	2.05	0.57
1:A:349:VAL:CG1	2:B:1453:PHE:HB2	2.35	0.57
3:C:851:ARG:HG3	3:C:851:ARG:NH2	2.19	0.57
1:A:84:ASN:HD21	1:A:86:ASN:HB3	1.69	0.57
1:D:201:GLU:CD	3:F:829:THR:H	2.13	0.57
1:D:227:LEU:HD12	1:D:227:LEU:O	2.04	0.57
3:I:851:ARG:HG3	3:I:851:ARG:NH2	2.19	0.57
1:D:305:ILE:HD12	1:D:305:ILE:N	2.20	0.57
1:D:352:GLU:HG3	1:D:353:ARG:N	2.19	0.57
1:A:233:MET:HE3	2:B:1443:MET:HE1	1.87	0.57
1:D:387:MET:HE3	1:D:391:SER:HB3	1.87	0.57
1:D:429:ILE:O	1:D:436:ASN:HB2	2.05	0.57
1:D:441:SER:CB	1:D:444:THR:HB	2.35	0.57
1:D:451:SER:O	1:D:452:SER:HB3	2.04	0.57
3:F:815:LEU:C	3:F:817:ARG:H	2.12	0.57
3:F:864:LYS:HE3	3:F:876:LYS:CE	2.34	0.57
1:G:121:VAL:HG12	1:G:122:GLY:N	2.20	0.57
1:A:189:LYS:HG2	1:A:304:THR:HG21	1.87	0.56
3:C:864:LYS:HE3	3:C:876:LYS:CE	2.31	0.56
1:D:48:VAL:HG12	1:D:48:VAL:O	2.04	0.56
2:E:1432:LYS:CG	2:E:1433:GLY:N	2.66	0.56
3:I:775:ILE:HD11	3:I:799:VAL:HG21	1.87	0.56
1:A:451:SER:O	1:A:452:SER:HB3	2.04	0.56
1:D:253:LEU:O	1:D:257:SER:HB2	2.05	0.56
1:D:297:TYR:CE2	1:D:321:ASP:HB3	2.40	0.56
1:D:376:ILE:O	1:D:376:ILE:HG22	2.04	0.56
1:D:6:ARG:HG3	1:D:6:ARG:O	2.05	0.56
1:D:300:THR:HG22	1:D:301:ASN:OD1	2.05	0.56
1:G:429:ILE:O	1:G:436:ASN:HB2	2.05	0.56
1:D:21:GLN:O	1:D:22:SER:C	2.48	0.56
1:G:21:GLN:O	1:G:22:SER:C	2.48	0.56
1:G:175:LEU:CD1	3:I:797:LYS:HD3	2.36	0.56
1:G:441:SER:CB	1:G:444:THR:HB	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:815:LEU:C	3:I:817:ARG:H	2.14	0.56
3:I:864:LYS:HE3	3:I:876:LYS:CE	2.33	0.56
3:F:781:VAL:HG22	3:F:817:ARG:HH11	1.70	0.56
1:A:255:PHE:HD2	1:A:335:MET:HE1	1.68	0.56
1:G:339:VAL:HG11	1:G:342:TYR:CD1	2.41	0.56
1:A:431:TRP:O	1:A:434:GLN:HB2	2.05	0.56
1:G:387:MET:HE3	1:G:391:SER:HB3	1.86	0.56
1:A:356:LEU:O	1:A:358:ARG:HG3	2.05	0.56
1:A:358:ARG:HD3	1:A:377:SER:HB3	1.88	0.56
3:C:781:VAL:HG22	3:C:817:ARG:HH11	1.71	0.56
1:D:226:ILE:HG23	1:D:227:LEU:N	2.20	0.56
1:G:53:LEU:HD13	1:G:54:TYR:N	2.21	0.56
1:G:320:ASP:C	1:G:322:GLY:H	2.14	0.56
3:I:781:VAL:HG22	3:I:817:ARG:HH11	1.70	0.56
3:I:798:GLU:HG2	3:I:799:VAL:N	2.21	0.56
1:A:21:GLN:O	1:A:22:SER:C	2.49	0.56
1:A:233:MET:HE3	2:B:1443:MET:CE	2.36	0.56
1:D:238:ASP:CG	1:D:239:SER:N	2.63	0.56
3:F:798:GLU:HG2	3:F:799:VAL:N	2.21	0.56
1:G:335:MET:HE2	1:G:337:TRP:CH2	2.41	0.56
1:D:401:ASP:OD1	1:D:404:PRO:HD3	2.06	0.55
1:G:352:GLU:HG3	1:G:353:ARG:N	2.20	0.55
1:G:358:ARG:HD3	1:G:377:SER:HB3	1.87	0.55
1:G:387:MET:CE	1:G:391:SER:HB3	2.36	0.55
1:A:297:TYR:CE2	1:A:321:ASP:HB3	2.41	0.55
3:C:815:LEU:C	3:C:817:ARG:H	2.14	0.55
1:D:331:LEU:HB3	1:D:345:ASN:OD1	2.06	0.55
3:I:742:TYR:O	3:I:743:THR:HG23	2.06	0.55
3:I:864:LYS:HB3	3:I:874:VAL:HG23	1.88	0.55
1:G:119:GLU:OE1	1:G:146:LYS:NZ	2.40	0.55
1:G:356:LEU:O	1:G:358:ARG:HG3	2.06	0.55
1:A:48:VAL:HG12	1:A:48:VAL:O	2.07	0.55
1:A:199:THR:O	1:A:202:GLY:N	2.39	0.55
3:C:866:TYR:O	3:C:868:PRO:HD3	2.07	0.55
1:D:142:ILE:HG23	1:D:156:ILE:CD1	2.34	0.55
1:D:237:LEU:HD21	1:D:249:VAL:HB	1.88	0.55
1:A:90:VAL:HG11	1:A:156:ILE:HD13	1.89	0.55
1:A:247:ARG:HG2	1:A:247:ARG:NH1	2.13	0.55
1:A:387:MET:CE	1:A:391:SER:HB3	2.36	0.55
3:F:742:TYR:CD1	3:F:742:TYR:C	2.85	0.55
1:G:156:ILE:HG22	1:G:157:LEU:HD23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:866:TYR:O	3:I:868:PRO:HD3	2.07	0.55
1:A:320:ASP:C	1:A:322:GLY:H	2.14	0.55
1:A:352:GLU:HG3	1:A:353:ARG:N	2.22	0.55
3:C:745:PRO:HB2	3:C:749:ASP:HB3	1.89	0.55
3:C:775:ILE:HD11	3:C:799:VAL:HG21	1.89	0.55
3:F:801:VAL:O	3:F:802:TYR:HB2	2.07	0.55
1:G:344:TYR:CZ	1:G:345:ASN:ND2	2.75	0.55
1:A:53:LEU:HD13	1:A:54:TYR:N	2.22	0.55
1:A:174:GLY:HA2	3:C:873:TRP:HH2	1.69	0.55
1:A:227:LEU:O	1:A:227:LEU:HD12	2.07	0.55
3:C:742:TYR:CD1	3:C:742:TYR:C	2.84	0.55
1:G:134:PRO:HD2	1:G:187:PHE:CE1	2.42	0.55
3:C:801:VAL:O	3:C:802:TYR:HB2	2.07	0.55
1:D:343:VAL:HG11	3:F:834:ARG:NH2	2.22	0.55
3:F:866:TYR:O	3:F:868:PRO:HD3	2.06	0.55
1:G:84:ASN:HD21	1:G:86:ASN:HB3	1.71	0.55
1:A:210:PRO:CG	1:A:335:MET:HE3	2.36	0.54
3:F:769:ARG:NH1	3:F:772:TYR:HE1	2.05	0.54
1:G:145:LEU:HD22	1:G:185:LEU:HD13	1.89	0.54
1:D:28:SER:O	1:D:29:SER:HB2	2.07	0.54
1:D:356:LEU:O	1:D:358:ARG:HG3	2.06	0.54
1:G:401:ASP:OD1	1:G:404:PRO:HD3	2.07	0.54
2:H:1450:GLY:O	2:H:1454:LYS:HG3	2.07	0.54
1:A:401:ASP:OD1	1:A:404:PRO:HD3	2.08	0.54
1:D:189:LYS:HZ1	1:D:304:THR:HB	1.72	0.54
1:A:300:THR:HG22	1:A:301:ASN:OD1	2.08	0.54
1:D:84:ASN:HD21	1:D:86:ASN:HB3	1.73	0.54
1:D:189:LYS:HG2	1:D:304:THR:HG21	1.89	0.54
1:D:208:PHE:CE1	1:D:281:VAL:HG22	2.42	0.54
1:G:79:LEU:HD12	1:G:139:ASP:HB2	1.89	0.54
3:C:798:GLU:HG2	3:C:799:VAL:N	2.22	0.54
1:D:34:ARG:HH21	1:D:95:TRP:NE1	2.06	0.54
1:D:250:ILE:CG2	2:H:1441:LEU:HG	2.37	0.54
1:D:420:ILE:HD12	1:D:420:ILE:O	2.07	0.54
3:I:745:PRO:HB2	3:I:749:ASP:HB3	1.89	0.54
1:A:441:SER:CB	1:A:444:THR:HB	2.37	0.54
1:D:29:SER:HB3	1:D:34:ARG:HB2	1.89	0.54
1:D:156:ILE:HG22	1:D:157:LEU:HD23	1.90	0.54
1:D:408:LEU:HD23	1:D:409:LYS:H	1.71	0.54
1:A:168:LYS:HB3	1:A:169:PRO:CD	2.38	0.54
1:A:429:ILE:O	1:A:436:ASN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:745:PRO:HB2	3:F:749:ASP:HB3	1.90	0.54
1:A:250:ILE:HG21	2:E:1441:LEU:HG	1.89	0.53
1:A:343:VAL:HG12	1:A:343:VAL:O	2.08	0.53
1:D:344:TYR:CZ	1:D:345:ASN:ND2	2.76	0.53
1:G:199:THR:O	1:G:202:GLY:N	2.39	0.53
1:A:24:ARG:HG2	1:A:39:GLN:HG3	1.90	0.53
2:B:1432:LYS:HD2	2:B:1432:LYS:O	2.08	0.53
1:D:197:LEU:HD21	1:D:299:ALA:HB1	1.90	0.53
3:F:738:LYS:HB2	3:F:741:TYR:HD2	1.73	0.53
1:D:210:PRO:HD3	1:D:335:MET:HG2	1.89	0.53
1:D:405:LEU:HB3	2:E:1452:PHE:HE1	1.72	0.53
1:A:174:GLY:CA	3:C:859:GLN:HE22	2.21	0.53
1:A:379:ASN:HA	1:A:420:ILE:O	2.08	0.53
1:D:199:THR:O	1:D:200:THR:C	2.51	0.53
1:G:376:ILE:HG22	1:G:376:ILE:O	2.07	0.53
1:A:210:PRO:HD3	1:A:335:MET:HG2	1.88	0.53
3:C:777:PHE:CD1	3:C:819:ALA:HB2	2.42	0.53
1:G:199:THR:O	1:G:200:THR:C	2.51	0.53
1:A:238:ASP:CG	1:A:239:SER:H	2.16	0.53
1:G:34:ARG:HH21	1:G:95:TRP:NE1	2.06	0.53
1:A:176:ASP:HB3	3:C:798:GLU:OE2	2.09	0.53
1:G:48:VAL:HG12	1:G:48:VAL:O	2.08	0.53
1:G:227:LEU:HD12	1:G:227:LEU:O	2.08	0.53
1:G:298:THR:HG22	1:G:299:ALA:N	2.23	0.53
3:I:742:TYR:CD1	3:I:742:TYR:C	2.86	0.53
1:A:430:ASN:HA	1:A:434:GLN:O	2.09	0.53
1:D:169:PRO:CA	1:D:178:ARG:HH11	2.19	0.53
3:F:742:TYR:O	3:F:743:THR:HG23	2.09	0.53
1:G:17:LEU:O	1:G:17:LEU:CD1	2.57	0.53
1:G:305:ILE:N	1:G:305:ILE:HD12	2.24	0.53
1:A:417:ILE:HG23	1:A:448:GLN:OE1	2.09	0.53
1:D:92:GLU:HB2	1:D:111:ILE:CD1	2.39	0.53
1:D:307:ILE:HG12	1:D:312:ASN:O	2.09	0.53
1:G:226:ILE:HG23	1:G:227:LEU:N	2.24	0.53
1:A:147:GLU:C	1:A:149:ASP:H	2.16	0.53
1:A:237:LEU:HD22	1:A:241:THR:HG21	1.89	0.53
1:A:451:SER:O	1:A:452:SER:CB	2.57	0.53
1:D:408:LEU:HD23	1:D:409:LYS:N	2.24	0.53
3:F:828:PRO:HB3	3:F:848:TYR:CE1	2.43	0.53
1:A:446:THR:HG22	1:A:447:PHE:N	2.24	0.52
1:D:17:LEU:O	1:D:17:LEU:CD1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:MET:CE	1:D:391:SER:HB3	2.39	0.52
1:G:169:PRO:CA	1:G:178:ARG:HH11	2.14	0.52
1:G:379:ASN:HA	1:G:420:ILE:O	2.09	0.52
3:I:777:PHE:CD1	3:I:819:ALA:HB2	2.44	0.52
1:A:121:VAL:CG1	1:A:122:GLY:H	2.14	0.52
3:I:777:PHE:CE2	3:I:815:LEU:HD11	2.44	0.52
1:A:405:LEU:HB3	2:B:1452:PHE:CE1	2.44	0.52
1:G:446:THR:HG22	1:G:447:PHE:N	2.24	0.52
1:A:329:LYS:HE2	1:A:333:MET:HG3	1.90	0.52
1:D:147:GLU:C	1:D:149:ASP:H	2.17	0.52
1:D:335:MET:HE2	1:D:337:TRP:CH2	2.44	0.52
1:D:431:TRP:O	1:D:434:GLN:HB2	2.09	0.52
1:A:293:GLU:O	1:A:295:TYR:N	2.43	0.52
3:F:869:GLU:H	3:F:869:GLU:CD	2.17	0.52
1:G:238:ASP:OD1	1:G:238:ASP:N	2.43	0.52
1:D:199:THR:O	1:D:202:GLY:N	2.43	0.52
3:F:775:ILE:HD11	3:F:799:VAL:HG21	1.89	0.52
1:G:57:LEU:HD11	1:G:106:GLN:HG3	1.91	0.52
1:G:147:GLU:C	1:G:149:ASP:H	2.18	0.52
1:G:233:MET:HE3	2:H:1443:MET:HE1	1.92	0.52
1:A:376:ILE:O	1:A:376:ILE:HG22	2.09	0.52
1:D:227:LEU:HD21	2:H:1432:LYS:HE3	1.91	0.52
1:G:6:ARG:HG3	1:G:431:TRP:HZ3	1.75	0.52
3:I:738:LYS:HB2	3:I:741:TYR:HD2	1.74	0.52
1:A:137:TYR:CE2	1:A:269:LYS:HD3	2.45	0.52
1:A:199:THR:O	1:A:200:THR:C	2.53	0.52
3:C:783:LEU:HD12	3:C:783:LEU:N	2.25	0.52
1:D:358:ARG:HD3	1:D:377:SER:HB3	1.92	0.52
3:F:816:ASN:ND2	3:F:879:HIS:HB2	2.25	0.52
1:G:176:ASP:HB2	1:G:178:ARG:CG	2.40	0.52
1:A:298:THR:HG22	1:A:299:ALA:N	2.25	0.52
3:C:778:GLU:HG2	3:C:779:GLY:N	2.24	0.52
3:F:777:PHE:CD1	3:F:819:ALA:HB2	2.44	0.52
1:D:379:ASN:HA	1:D:420:ILE:O	2.10	0.51
3:F:864:LYS:HB3	3:F:874:VAL:HG23	1.91	0.51
1:G:57:LEU:HD13	1:G:100:VAL:CG1	2.39	0.51
1:A:216:LEU:HB3	1:A:270:VAL:CG1	2.40	0.51
1:A:420:ILE:O	1:A:420:ILE:HD12	2.10	0.51
3:C:864:LYS:HB3	3:C:874:VAL:HG23	1.91	0.51
1:G:358:ARG:HH11	1:G:358:ARG:HG2	1.74	0.51
1:A:137:TYR:OH	1:A:267:PHE:HD2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:TYR:CZ	1:A:345:ASN:ND2	2.78	0.51
1:D:255:PHE:HD2	1:D:335:MET:HE1	1.75	0.51
3:F:783:LEU:N	3:F:783:LEU:HD12	2.25	0.51
1:G:233:MET:HE2	1:G:233:MET:HA	1.92	0.51
1:G:380:ILE:CG2	1:G:381:ILE:N	2.71	0.51
3:I:801:VAL:O	3:I:802:TYR:HB2	2.09	0.51
1:D:380:ILE:CG2	1:D:381:ILE:N	2.70	0.51
1:G:45:TRP:CH2	1:G:100:VAL:HG21	2.40	0.51
1:A:27:PHE:CZ	1:A:71:VAL:HG23	2.39	0.51
1:G:216:LEU:HB3	1:G:270:VAL:HG12	1.93	0.51
1:G:380:ILE:CG2	1:G:381:ILE:H	2.23	0.51
3:I:816:ASN:ND2	3:I:879:HIS:HB2	2.25	0.51
1:A:25:TYR:HD2	1:A:425:ASN:HD22	1.58	0.51
3:C:754:THR:HG23	3:C:754:THR:O	2.10	0.51
1:D:266:ARG:HB2	1:D:267:PHE:HD1	1.76	0.51
1:G:166:LEU:HD12	1:G:211:PHE:CE1	2.46	0.51
1:A:34:ARG:HH21	1:A:95:TRP:NE1	2.09	0.51
1:A:174:GLY:H	3:C:859:GLN:CD	2.18	0.51
1:A:444:THR:HG22	1:A:445:LEU:N	2.25	0.51
3:I:843:LEU:HD23	3:I:868:PRO:HB3	1.92	0.51
1:A:6:ARG:CG	1:A:431:TRP:HH2	2.24	0.51
1:A:274:LYS:HG3	1:A:275:GLU:OE2	2.11	0.51
1:A:297:TYR:HD1	1:A:297:TYR:H	1.59	0.51
3:C:738:LYS:HB2	3:C:741:TYR:HD2	1.74	0.51
1:G:274:LYS:O	1:G:277:ARG:HB2	2.10	0.51
2:B:1450:GLY:O	2:B:1454:LYS:HG3	2.11	0.51
1:D:173:PHE:HA	3:F:859:GLN:OE1	2.09	0.51
1:G:26:ILE:HD13	1:G:438:ALA:CB	2.41	0.51
1:G:274:LYS:HG3	1:G:275:GLU:OE2	2.11	0.51
1:G:307:ILE:HG12	1:G:312:ASN:O	2.10	0.51
1:G:451:SER:O	1:G:452:SER:CB	2.58	0.51
3:C:737:THR:O	3:C:738:LYS:O	2.29	0.51
1:D:358:ARG:HG2	1:D:358:ARG:HH11	1.75	0.51
3:I:795:ARG:HH21	3:I:800:ILE:HD11	1.75	0.51
1:A:36:VAL:HG11	1:A:80:LEU:HD11	1.92	0.50
3:C:777:PHE:CE2	3:C:815:LEU:HD11	2.46	0.50
3:C:797:LYS:HG2	3:C:826:VAL:HG22	1.93	0.50
1:G:420:ILE:O	1:G:420:ILE:HD12	2.11	0.50
3:I:767:ILE:HD11	3:I:792:VAL:HG11	1.94	0.50
1:A:119:GLU:O	1:A:120:GLU:C	2.53	0.50
1:A:188:SER:HB2	1:A:193:THR:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:787:ASN:O	3:C:791:ILE:HG13	2.10	0.50
1:D:145:LEU:HD22	1:D:185:LEU:HD13	1.93	0.50
1:D:380:ILE:CG2	1:D:381:ILE:H	2.24	0.50
3:F:767:ILE:HD11	3:F:792:VAL:HG11	1.93	0.50
3:F:787:ASN:O	3:F:791:ILE:HG13	2.11	0.50
1:G:175:LEU:HD13	3:I:797:LYS:HD3	1.92	0.50
1:A:189:LYS:HG2	1:A:304:THR:CG2	2.40	0.50
1:G:137:TYR:CE2	1:G:269:LYS:HD3	2.46	0.50
1:G:417:ILE:HG23	1:G:448:GLN:OE1	2.11	0.50
3:I:737:THR:O	3:I:738:LYS:O	2.29	0.50
1:A:274:LYS:O	1:A:277:ARG:HB2	2.12	0.50
3:C:767:ILE:HD11	3:C:792:VAL:HG11	1.93	0.50
1:D:125:SER:OG	1:D:147:GLU:HB2	2.12	0.50
1:D:200:THR:O	3:F:851:ARG:HB3	2.11	0.50
3:I:783:LEU:N	3:I:783:LEU:HD12	2.25	0.50
3:I:869:GLU:H	3:I:869:GLU:CD	2.20	0.50
1:A:179:VAL:HG23	1:A:281:VAL:HG21	1.93	0.50
1:A:328:PHE:HB2	1:A:351:ILE:HD11	1.94	0.50
1:A:335:MET:HE2	1:A:337:TRP:CH2	2.46	0.50
1:D:451:SER:O	1:D:452:SER:CB	2.59	0.50
2:E:1450:GLY:O	2:E:1454:LYS:HG3	2.11	0.50
3:F:821:VAL:HB	3:F:875:PHE:CE1	2.47	0.50
1:G:36:VAL:HG11	1:G:80:LEU:HD11	1.94	0.50
1:G:84:ASN:OD1	1:G:87:GLU:HG2	2.11	0.50
1:A:255:PHE:CE2	1:A:335:MET:HE1	2.47	0.50
3:C:816:ASN:ND2	3:C:879:HIS:HB2	2.26	0.50
1:D:201:GLU:OE2	3:F:828:PRO:HA	2.12	0.50
1:D:430:ASN:HA	1:D:434:GLN:O	2.12	0.50
1:D:446:THR:HG22	1:D:447:PHE:N	2.26	0.50
1:A:339:VAL:HG11	1:A:342:TYR:CD1	2.46	0.50
1:D:239:SER:O	1:D:241:THR:N	2.45	0.50
1:D:343:VAL:HG12	1:D:343:VAL:O	2.12	0.50
1:G:27:PHE:CZ	1:G:71:VAL:HG23	2.37	0.50
3:I:787:ASN:O	3:I:791:ILE:HG13	2.11	0.50
3:I:797:LYS:HG2	3:I:826:VAL:HG22	1.93	0.50
3:C:828:PRO:HB3	3:C:848:TYR:CE1	2.47	0.50
1:D:343:VAL:CG1	3:F:834:ARG:CZ	2.90	0.50
3:F:777:PHE:CE2	3:F:815:LEU:HD11	2.47	0.50
3:I:772:TYR:CE2	3:I:796:ARG:NH2	2.80	0.50
1:A:142:ILE:HG12	1:A:156:ILE:HG13	1.94	0.49
1:A:175:LEU:HD12	3:C:797:LYS:HD3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:HE3	1:A:332:GLU:OE1	2.12	0.49
3:C:810:PRO:HD2	3:C:813:GLU:HG3	1.94	0.49
1:G:6:ARG:HG3	1:G:431:TRP:CZ3	2.47	0.49
1:D:84:ASN:C	1:D:86:ASN:H	2.20	0.49
1:G:358:ARG:HG2	1:G:358:ARG:NH1	2.27	0.49
1:G:372:LYS:HG2	1:G:385:ASN:OD1	2.12	0.49
1:A:92:GLU:HB2	1:A:111:ILE:CD1	2.41	0.49
3:F:767:ILE:CG1	3:F:768:GLY:H	2.25	0.49
1:A:233:MET:HE2	1:A:233:MET:HA	1.95	0.49
1:D:149:ASP:HB2	1:D:178:ARG:NH2	2.27	0.49
3:F:795:ARG:HH21	3:F:800:ILE:HD11	1.77	0.49
3:I:802:TYR:CE1	3:I:809:PRO:HD2	2.47	0.49
3:I:828:PRO:HB3	3:I:848:TYR:CE1	2.47	0.49
1:D:297:TYR:HD1	1:D:297:TYR:H	1.58	0.49
3:F:767:ILE:CG1	3:F:768:GLY:N	2.74	0.49
1:G:233:MET:HE3	2:H:1443:MET:CE	2.43	0.49
1:G:444:THR:HG22	1:G:445:LEU:N	2.27	0.49
3:C:742:TYR:O	3:C:743:THR:HG23	2.12	0.49
1:D:421:GLU:OE1	1:D:422:ARG:HG2	2.13	0.49
3:F:742:TYR:HD1	3:F:743:THR:N	2.10	0.49
3:F:754:THR:HG23	3:F:754:THR:O	2.12	0.49
1:G:7:LEU:C	1:G:9:ALA:N	2.68	0.49
1:G:53:LEU:HD13	1:G:54:TYR:O	2.13	0.49
3:C:742:TYR:HD1	3:C:743:THR:N	2.11	0.49
1:D:216:LEU:HB3	1:D:270:VAL:CG1	2.42	0.49
1:G:297:TYR:HD1	1:G:297:TYR:H	1.58	0.49
3:C:869:GLU:H	3:C:869:GLU:CD	2.21	0.49
3:F:778:GLU:HG2	3:F:779:GLY:N	2.27	0.49
3:F:805:ASP:HA	3:F:808:LYS:CB	2.42	0.49
1:A:17:LEU:O	1:A:17:LEU:CD1	2.60	0.49
1:A:42:ILE:HD11	1:A:58:ASN:HD22	1.78	0.49
1:A:156:ILE:HG22	1:A:157:LEU:HD23	1.94	0.49
1:D:53:LEU:HD13	1:D:54:TYR:O	2.13	0.49
1:D:234:TYR:HA	1:D:237:LEU:CD1	2.42	0.49
1:G:34:ARG:HH21	1:G:95:TRP:CD1	2.30	0.49
1:G:137:TYR:CE2	1:G:138:ARG:HG3	2.48	0.49
3:I:754:THR:O	3:I:754:THR:HG23	2.13	0.49
3:I:778:GLU:HG2	3:I:779:GLY:N	2.27	0.49
3:I:821:VAL:HB	3:I:875:PHE:CE1	2.48	0.49
1:A:238:ASP:OD2	1:A:240:THR:N	2.36	0.49
3:C:805:ASP:HA	3:C:808:LYS:CB	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:772:TYR:CE2	3:F:796:ARG:NH2	2.81	0.49
1:A:84:ASN:C	1:A:86:ASN:H	2.20	0.48
1:A:216:LEU:HB2	1:A:272:ILE:CD1	2.43	0.48
1:A:408:LEU:HD23	1:A:409:LYS:N	2.28	0.48
3:C:795:ARG:HH21	3:C:800:ILE:HD11	1.78	0.48
1:A:137:TYR:CD1	1:A:269:LYS:HB3	2.48	0.48
1:A:189:LYS:NZ	1:A:304:THR:HB	2.29	0.48
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.77	0.48
3:C:750:LEU:HA	3:C:753:ILE:HD11	1.94	0.48
1:A:50:THR:HG22	1:A:51:ASP:N	2.27	0.48
1:A:295:TYR:HH	3:C:831:LYS:H	1.60	0.48
3:C:742:TYR:C	3:C:742:TYR:HD1	2.21	0.48
1:D:444:THR:HG22	1:D:445:LEU:N	2.28	0.48
1:G:24:ARG:NH2	1:G:443:LYS:O	2.46	0.48
1:G:293:GLU:O	1:G:295:TYR:N	2.46	0.48
3:I:742:TYR:HD1	3:I:743:THR:N	2.11	0.48
1:A:92:GLU:HB2	1:A:111:ILE:HD12	1.94	0.48
1:D:50:THR:HG22	1:D:51:ASP:N	2.28	0.48
1:A:384:VAL:HG13	1:A:414:LEU:CD1	2.37	0.48
1:D:164:ILE:HD12	1:D:277:ARG:CZ	2.44	0.48
1:D:343:VAL:CG1	3:F:834:ARG:NH1	2.77	0.48
1:G:255:PHE:CE2	1:G:335:MET:HE1	2.47	0.48
1:A:119:GLU:O	1:A:124:LYS:CE	2.61	0.48
1:D:34:ARG:HH21	1:D:95:TRP:CD1	2.31	0.48
1:D:349:VAL:CG1	2:E:1453:PHE:HB2	2.41	0.48
1:G:216:LEU:HB2	1:G:272:ILE:HD12	1.94	0.48
3:I:810:PRO:HD2	3:I:813:GLU:HG3	1.94	0.48
1:A:53:LEU:HD13	1:A:54:TYR:O	2.14	0.48
1:A:175:LEU:O	3:C:798:GLU:HB2	2.14	0.48
3:C:767:ILE:CG1	3:C:768:GLY:H	2.26	0.48
1:D:356:LEU:C	1:D:358:ARG:H	2.22	0.48
3:F:797:LYS:HG2	3:F:826:VAL:HG22	1.96	0.48
1:G:7:LEU:O	1:G:9:ALA:N	2.46	0.48
1:G:84:ASN:C	1:G:86:ASN:H	2.20	0.48
3:I:767:ILE:CG1	3:I:768:GLY:N	2.77	0.48
1:A:358:ARG:HG2	1:A:358:ARG:NH1	2.29	0.48
1:A:358:ARG:NH1	1:A:380:ILE:HD12	2.28	0.48
1:A:380:ILE:CG2	1:A:381:ILE:N	2.72	0.48
3:C:769:ARG:NH1	3:C:772:TYR:CE1	2.81	0.48
1:D:356:LEU:O	1:D:358:ARG:N	2.46	0.48
3:F:742:TYR:C	3:F:742:TYR:HD1	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:O	1:A:178:ARG:HD2	2.14	0.48
3:C:767:ILE:CG1	3:C:768:GLY:N	2.74	0.48
1:D:188:SER:HB2	1:D:193:THR:HB	1.96	0.48
1:G:112:PHE:CB	1:G:156:ILE:HG23	2.36	0.48
1:G:176:ASP:HB2	1:G:178:ARG:HG2	1.96	0.48
1:A:84:ASN:OD1	1:A:87:GLU:HG2	2.13	0.48
1:D:54:TYR:CD1	1:D:54:TYR:C	2.91	0.48
1:G:24:ARG:HG2	1:G:39:GLN:HG3	1.96	0.48
1:A:179:VAL:CG2	1:A:281:VAL:HG11	2.44	0.47
1:D:13:PHE:HE1	1:D:26:ILE:HD12	1.79	0.47
1:D:293:GLU:O	1:D:295:TYR:N	2.47	0.47
3:F:828:PRO:HB3	3:F:848:TYR:CD1	2.49	0.47
1:G:33:THR:HG23	1:G:49:LEU:HG	1.96	0.47
1:G:248:ASN:HD21	1:G:339:VAL:HG21	1.78	0.47
1:A:275:GLU:CD	1:A:275:GLU:N	2.72	0.47
1:A:295:TYR:HB3	3:C:846:ILE:HG22	1.95	0.47
3:C:772:TYR:CE2	3:C:796:ARG:NH2	2.82	0.47
1:D:189:LYS:HG2	1:D:304:THR:CG2	2.44	0.47
3:F:737:THR:O	3:F:738:LYS:O	2.32	0.47
1:G:50:THR:HG22	1:G:51:ASP:N	2.29	0.47
1:D:384:VAL:HG13	1:D:414:LEU:CD1	2.37	0.47
3:F:791:ILE:HG23	3:F:802:TYR:CE2	2.50	0.47
1:G:168:LYS:O	1:G:178:ARG:HD2	2.14	0.47
1:G:238:ASP:OD2	1:G:240:THR:CG2	2.61	0.47
3:I:769:ARG:NH1	3:I:772:TYR:CE1	2.82	0.47
1:A:33:THR:HG23	1:A:49:LEU:HG	1.97	0.47
1:D:329:LYS:HE2	1:D:333:MET:HG3	1.95	0.47
3:F:810:PRO:HD2	3:F:813:GLU:HG3	1.95	0.47
1:G:343:VAL:CG1	3:I:834:ARG:CZ	2.92	0.47
1:A:372:LYS:HG2	1:A:385:ASN:OD1	2.13	0.47
3:C:843:LEU:HD23	3:C:868:PRO:HB3	1.95	0.47
1:D:343:VAL:CG1	3:F:834:ARG:NH2	2.77	0.47
3:F:847:ASN:CG	3:F:847:ASN:O	2.57	0.47
1:G:91:MET:HA	1:G:109:PHE:O	2.14	0.47
2:H:1434:PHE:CD1	2:H:1435:LYS:N	2.78	0.47
1:D:82:LEU:N	1:D:82:LEU:HD12	2.29	0.47
1:D:119:GLU:O	1:D:120:GLU:C	2.57	0.47
3:F:791:ILE:HG21	3:F:815:LEU:HD23	1.97	0.47
3:F:802:TYR:CE1	3:F:809:PRO:HD2	2.50	0.47
1:G:275:GLU:CD	1:G:275:GLU:N	2.73	0.47
1:A:266:ARG:HB2	1:A:267:PHE:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:791:ILE:HG21	3:C:815:LEU:HD23	1.97	0.47
3:C:848:TYR:CE2	3:C:852:LEU:HD22	2.50	0.47
1:D:189:LYS:N	1:D:313:GLU:OE1	2.42	0.47
3:I:828:PRO:HB3	3:I:848:TYR:CD1	2.50	0.47
1:A:290:PHE:CE2	3:C:831:LYS:HD2	2.49	0.47
1:A:356:LEU:C	1:A:358:ARG:H	2.22	0.47
1:A:421:GLU:OE1	1:A:422:ARG:HG2	2.15	0.47
3:C:766:THR:HG22	3:C:767:ILE:N	2.29	0.47
1:D:417:ILE:HG23	1:D:448:GLN:OE1	2.15	0.47
3:F:818:LYS:NZ	3:F:818:LYS:HB3	2.30	0.47
3:I:767:ILE:CG1	3:I:768:GLY:H	2.27	0.47
3:C:809:PRO:CB	3:C:814:GLY:H	2.28	0.47
1:D:27:PHE:CZ	1:D:71:VAL:HG23	2.41	0.47
1:D:358:ARG:HG2	1:D:358:ARG:NH1	2.29	0.47
1:G:38:ILE:HG12	1:G:43:ILE:HG12	1.97	0.47
1:G:92:GLU:HB2	1:G:111:ILE:CD1	2.45	0.47
1:G:121:VAL:CG1	1:G:122:GLY:H	2.25	0.47
1:G:328:PHE:HB2	1:G:351:ILE:HD11	1.96	0.47
1:A:310:GLY:O	1:A:312:ASN:N	2.48	0.46
1:A:408:LEU:HD23	1:A:409:LYS:H	1.78	0.46
3:C:749:ASP:O	3:C:753:ILE:HG13	2.15	0.46
3:C:818:LYS:HB3	3:C:818:LYS:NZ	2.30	0.46
1:D:90:VAL:HB	1:D:112:PHE:HB3	1.96	0.46
1:D:234:TYR:HA	1:D:237:LEU:HD12	1.96	0.46
1:D:298:THR:HG22	1:D:299:ALA:H	1.80	0.46
1:G:61:ARG:NH2	1:G:103:VAL:HG13	2.30	0.46
1:G:188:SER:HB2	1:G:193:THR:HB	1.97	0.46
1:G:228:ASN:O	1:G:229:LYS:C	2.58	0.46
1:G:266:ARG:HB2	1:G:267:PHE:HD1	1.80	0.46
1:G:384:VAL:HG13	1:G:414:LEU:CD1	2.36	0.46
1:A:380:ILE:CG2	1:A:381:ILE:H	2.25	0.46
3:C:791:ILE:HG23	3:C:802:TYR:CE2	2.50	0.46
1:D:6:ARG:O	1:D:6:ARG:CG	2.63	0.46
1:D:115:SER:O	1:D:118:GLU:HG3	2.16	0.46
3:F:833:SER:O	3:F:834:ARG:HG2	2.15	0.46
3:F:749:ASP:O	3:F:753:ILE:HG13	2.16	0.46
3:F:766:THR:HG22	3:F:767:ILE:N	2.31	0.46
3:F:816:ASN:ND2	3:F:816:ASN:O	2.43	0.46
1:G:26:ILE:HD13	1:G:438:ALA:HB1	1.97	0.46
3:I:750:LEU:HA	3:I:753:ILE:HD11	1.97	0.46
3:I:809:PRO:CB	3:I:814:GLY:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ASN:ND2	1:A:342:TYR:CZ	2.82	0.46
1:A:356:LEU:O	1:A:358:ARG:N	2.47	0.46
1:D:233:MET:HE3	2:E:1443:MET:HE1	1.97	0.46
3:F:791:ILE:HG23	3:F:802:TYR:CD2	2.51	0.46
1:D:76:SER:OG	1:D:139:ASP:OD2	2.32	0.46
1:D:84:ASN:OD1	1:D:87:GLU:HG2	2.16	0.46
3:F:778:GLU:O	3:F:817:ARG:NH2	2.49	0.46
1:A:189:LYS:HZ1	1:A:304:THR:HB	1.79	0.46
1:G:71:VAL:CG1	1:G:82:LEU:HD23	2.46	0.46
1:G:297:TYR:CD2	1:G:321:ASP:HB3	2.51	0.46
1:A:90:VAL:HB	1:A:112:PHE:HB3	1.96	0.46
1:D:274:LYS:HG3	1:D:275:GLU:OE2	2.16	0.46
1:D:399:GLU:O	1:D:400:SER:HB2	2.15	0.46
3:C:753:ILE:HD12	3:C:753:ILE:C	2.41	0.46
3:C:802:TYR:CE1	3:C:809:PRO:HD2	2.50	0.46
1:D:134:PRO:HD2	1:D:187:PHE:CE1	2.51	0.46
1:G:116:ILE:C	1:G:118:GLU:H	2.24	0.46
1:G:166:LEU:HD12	1:G:211:PHE:HE1	1.81	0.46
3:I:749:ASP:O	3:I:753:ILE:HG13	2.16	0.46
3:I:778:GLU:O	3:I:817:ARG:NH2	2.49	0.46
1:D:372:LYS:HG2	1:D:385:ASN:OD1	2.15	0.46
2:E:1431:MET:HG3	2:E:1431:MET:O	2.16	0.46
3:F:734:ILE:HG22	3:F:747:MET:HE1	1.98	0.46
3:F:809:PRO:CB	3:F:814:GLY:H	2.28	0.46
1:G:288:ASN:OD1	3:I:832:THR:HB	2.16	0.46
1:G:343:VAL:HG12	1:G:343:VAL:O	2.15	0.46
3:I:791:ILE:HG23	3:I:802:TYR:CE2	2.51	0.46
3:I:833:SER:O	3:I:834:ARG:HG2	2.16	0.46
3:I:847:ASN:O	3:I:847:ASN:CG	2.59	0.46
1:A:34:ARG:HH21	1:A:95:TRP:CD1	2.35	0.45
1:A:223:LEU:O	1:A:226:ILE:HG22	2.16	0.45
3:F:750:LEU:HA	3:F:753:ILE:HD11	1.97	0.45
3:F:781:VAL:HG22	3:F:817:ARG:NH1	2.31	0.45
1:G:57:LEU:CD2	1:G:100:VAL:HG11	2.26	0.45
1:G:173:PHE:HA	3:I:859:GLN:OE1	2.16	0.45
1:G:216:LEU:HB2	1:G:272:ILE:HD11	1.98	0.45
1:G:310:GLY:O	1:G:312:ASN:N	2.49	0.45
3:C:841:ASP:N	3:C:841:ASP:OD2	2.49	0.45
3:C:734:ILE:HG22	3:C:747:MET:HE1	1.98	0.45
1:G:57:LEU:HD13	1:G:100:VAL:CB	2.47	0.45
1:G:356:LEU:C	1:G:358:ARG:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:408:LEU:HD23	1:G:409:LYS:N	2.31	0.45
1:D:234:TYR:C	1:D:236:SER:H	2.23	0.45
3:C:821:VAL:HB	3:C:875:PHE:CE1	2.51	0.45
1:G:314:ILE:HG23	1:G:327:LEU:O	2.17	0.45
1:G:370:LEU:O	1:G:372:LYS:HG3	2.17	0.45
1:A:343:VAL:HA	1:A:346:ASN:ND2	2.32	0.45
1:D:296:ASP:HB2	1:D:297:TYR:CD1	2.51	0.45
1:D:325:ILE:HD12	1:D:327:LEU:HD21	1.99	0.45
1:A:13:PHE:HE1	1:A:26:ILE:HD12	1.81	0.45
1:A:343:VAL:O	1:A:343:VAL:CG1	2.64	0.45
1:A:444:THR:CG2	1:A:445:LEU:N	2.79	0.45
3:C:791:ILE:HG23	3:C:802:TYR:CD2	2.51	0.45
1:D:250:ILE:O	1:D:254:GLN:HG3	2.16	0.45
1:D:282:GLN:HG2	1:D:342:TYR:HB3	1.99	0.45
1:D:358:ARG:NH1	1:D:380:ILE:HD12	2.31	0.45
3:I:742:TYR:C	3:I:742:TYR:HD1	2.24	0.45
3:I:791:ILE:HG21	3:I:815:LEU:HD23	1.99	0.45
1:A:71:VAL:CG1	1:A:82:LEU:HD23	2.47	0.45
3:C:828:PRO:HB3	3:C:848:TYR:CD1	2.51	0.45
1:D:189:LYS:NZ	1:D:304:THR:HB	2.31	0.45
1:G:53:LEU:HD22	1:G:54:TYR:H	1.82	0.45
1:A:7:LEU:O	1:A:9:ALA:N	2.47	0.45
1:A:107:ASP:C	1:A:109:PHE:N	2.75	0.45
1:A:242:ASP:OD1	1:A:244:ILE:N	2.50	0.45
1:G:13:PHE:HE1	1:G:26:ILE:HD12	1.82	0.45
1:G:296:ASP:HB2	1:G:297:TYR:CD1	2.52	0.45
3:I:791:ILE:HG23	3:I:802:TYR:CD2	2.51	0.45
1:A:54:TYR:CD1	1:A:54:TYR:C	2.95	0.45
1:A:395:LYS:C	1:A:397:ILE:N	2.74	0.45
1:A:443:LYS:H	1:A:443:LYS:CD	2.22	0.45
1:G:82:LEU:HD12	1:G:82:LEU:N	2.32	0.45
1:D:248:ASN:HD21	1:D:339:VAL:HG21	1.81	0.44
1:D:320:ASP:O	1:D:322:GLY:N	2.50	0.44
1:G:35:ILE:O	1:G:45:TRP:HA	2.16	0.44
1:G:197:LEU:HD21	1:G:299:ALA:HB1	1.99	0.44
1:D:69:PHE:HA	1:D:83:PHE:O	2.17	0.44
3:F:843:LEU:HD23	3:F:868:PRO:HB3	1.98	0.44
1:G:7:LEU:HD13	1:G:431:TRP:CG	2.52	0.44
1:G:173:PHE:O	3:I:799:VAL:HG12	2.16	0.44
1:G:443:LYS:H	1:G:443:LYS:CD	2.25	0.44
1:G:444:THR:CG2	1:G:445:LEU:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:805:ASP:HA	3:I:808:LYS:CB	2.42	0.44
1:A:370:LEU:O	1:A:372:LYS:HG3	2.18	0.44
3:C:818:LYS:HD2	3:C:818:LYS:N	2.28	0.44
1:G:373:LEU:HB3	1:G:384:VAL:HG23	1.98	0.44
1:D:24:ARG:HG2	1:D:39:GLN:HG3	1.99	0.44
1:D:138:ARG:O	1:D:139:ASP:C	2.61	0.44
3:F:848:TYR:CE2	3:F:852:LEU:HD22	2.52	0.44
1:G:408:LEU:HD23	1:G:409:LYS:H	1.81	0.44
3:I:734:ILE:HG22	3:I:747:MET:HE1	1.98	0.44
1:A:376:ILE:HD13	1:A:424:PRO:HD2	1.99	0.44
3:C:781:VAL:HG22	3:C:817:ARG:NH1	2.31	0.44
3:C:822:THR:HG23	3:C:874:VAL:CG1	2.47	0.44
1:D:19:ALA:C	1:D:21:GLN:N	2.75	0.44
1:G:358:ARG:NH1	1:G:380:ILE:HD12	2.32	0.44
1:G:369:GLN:OE1	1:G:450:ILE:HG21	2.18	0.44
3:I:818:LYS:NZ	3:I:818:LYS:HB3	2.33	0.44
1:D:223:LEU:O	1:D:226:ILE:HG22	2.18	0.44
1:D:295:TYR:O	3:F:846:ILE:HG22	2.17	0.44
1:G:54:TYR:CD1	1:G:54:TYR:C	2.95	0.44
3:I:768:GLY:HA2	3:I:794:ILE:CD1	2.48	0.44
1:D:198:ASN:OD1	1:D:198:ASN:C	2.60	0.44
3:F:753:ILE:HD12	3:F:753:ILE:C	2.42	0.44
3:F:783:LEU:O	3:F:785:ASN:N	2.51	0.44
3:F:841:ASP:OD2	3:F:841:ASP:N	2.50	0.44
1:G:216:LEU:HB3	1:G:270:VAL:HG13	1.99	0.44
3:C:737:THR:O	3:C:738:LYS:C	2.60	0.44
1:D:36:VAL:HG11	1:D:80:LEU:HD11	1.98	0.44
1:D:120:GLU:O	1:D:121:VAL:C	2.61	0.44
1:D:237:LEU:HD22	1:D:246:LYS:HA	1.99	0.44
1:G:156:ILE:C	1:G:157:LEU:HD23	2.43	0.44
1:G:349:VAL:CG1	2:H:1453:PHE:HB2	2.47	0.44
3:I:753:ILE:C	3:I:753:ILE:HD12	2.43	0.44
3:I:783:LEU:O	3:I:785:ASN:N	2.51	0.44
1:A:102:ASP:O	1:A:106:GLN:HB2	2.18	0.44
3:C:847:ASN:CG	3:C:847:ASN:O	2.58	0.44
1:D:274:LYS:O	1:D:277:ARG:HB2	2.17	0.44
1:D:370:LEU:O	1:D:372:LYS:HG3	2.18	0.44
1:G:228:ASN:O	1:G:231:LEU:N	2.51	0.44
1:G:421:GLU:OE1	1:G:422:ARG:HG2	2.18	0.44
1:G:437:LEU:HB2	1:G:450:ILE:HD11	2.00	0.44
1:A:82:LEU:N	1:A:82:LEU:HD12	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:804:ASP:CG	3:C:805:ASP:H	2.26	0.43
1:D:168:LYS:O	1:D:178:ARG:HD2	2.17	0.43
1:A:228:ASN:O	1:A:229:LYS:C	2.61	0.43
1:A:395:LYS:HD3	1:A:399:GLU:OE2	2.18	0.43
3:C:778:GLU:O	3:C:817:ARG:NH2	2.51	0.43
1:D:138:ARG:O	1:D:140:SER:N	2.51	0.43
1:G:7:LEU:C	1:G:9:ALA:H	2.26	0.43
1:G:93:VAL:HB	1:G:95:TRP:NE1	2.34	0.43
1:G:189:LYS:HA	1:G:189:LYS:HD3	1.87	0.43
1:A:176:ASP:CB	3:C:798:GLU:OE2	2.66	0.43
1:A:226:ILE:CG2	1:A:227:LEU:N	2.81	0.43
1:D:216:LEU:HB3	1:D:270:VAL:HG12	2.00	0.43
1:D:239:SER:C	1:D:241:THR:N	2.76	0.43
1:D:320:ASP:C	1:D:322:GLY:N	2.73	0.43
3:F:769:ARG:NH1	3:F:772:TYR:CE1	2.85	0.43
3:F:804:ASP:CG	3:F:805:ASP:H	2.26	0.43
1:G:343:VAL:HA	1:G:346:ASN:ND2	2.33	0.43
3:I:742:TYR:O	3:I:767:ILE:HG13	2.19	0.43
1:A:38:ILE:HG12	1:A:43:ILE:HG12	2.00	0.43
1:A:93:VAL:HB	1:A:95:TRP:HE1	1.83	0.43
1:A:373:LEU:HB3	1:A:384:VAL:HG23	2.00	0.43
1:A:383:GLN:O	1:A:383:GLN:HG2	2.18	0.43
1:D:92:GLU:HB2	1:D:111:ILE:HD12	2.00	0.43
1:D:247:ARG:NH2	1:D:338:ASP:OD2	2.52	0.43
1:D:395:LYS:C	1:D:397:ILE:N	2.76	0.43
3:I:841:ASP:OD2	3:I:841:ASP:N	2.51	0.43
1:A:379:ASN:O	1:A:419:THR:HA	2.19	0.43
1:D:10:LEU:HG	1:D:11:PRO:CD	2.47	0.43
1:D:71:VAL:CG1	1:D:82:LEU:HD23	2.49	0.43
1:D:395:LYS:O	1:D:397:ILE:N	2.51	0.43
1:D:444:THR:CG2	1:D:445:LEU:N	2.82	0.43
3:F:851:ARG:NH2	3:F:851:ARG:CG	2.80	0.43
1:G:19:ALA:C	1:G:21:GLN:N	2.76	0.43
3:C:762:VAL:HG22	3:C:763:SER:N	2.34	0.43
3:C:833:SER:O	3:C:834:ARG:HG2	2.18	0.43
1:D:39:GLN:O	1:D:40:ASP:C	2.61	0.43
1:D:255:PHE:CE2	1:D:335:MET:HE1	2.52	0.43
1:G:114:TYR:HA	1:G:118:GLU:OE2	2.18	0.43
1:G:134:PRO:HD2	1:G:187:PHE:CD1	2.53	0.43
1:G:189:LYS:HZ1	1:G:304:THR:HB	1.83	0.43
1:G:219:ASN:OD1	1:G:219:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:PRO:HB2	1:G:368:GLU:OE2	2.18	0.43
1:A:93:VAL:HB	1:A:95:TRP:NE1	2.33	0.43
1:A:116:ILE:C	1:A:118:GLU:H	2.26	0.43
3:C:875:PHE:CD1	3:C:875:PHE:C	2.97	0.43
1:D:321:ASP:OD1	1:D:323:SER:HB2	2.19	0.43
1:D:340:ASP:O	1:D:341:ASN:HB2	2.18	0.43
1:G:32:GLY:HA2	1:G:428:TYR:O	2.19	0.43
1:A:200:THR:O	3:C:851:ARG:HD2	2.19	0.43
3:F:875:PHE:CD1	3:F:875:PHE:C	2.97	0.43
1:G:190:ASP:OD1	1:G:192:LEU:N	2.47	0.43
1:G:206:PHE:CZ	1:G:284:PRO:HG3	2.54	0.43
1:G:304:THR:HG21	1:G:313:GLU:OE1	2.18	0.43
1:A:128:LYS:O	1:A:129:LYS:HB2	2.19	0.43
1:A:194:LEU:HB3	1:A:208:PHE:HB2	2.01	0.43
1:A:209:TYR:HA	1:A:210:PRO:HA	1.78	0.43
1:A:336:SER:HB2	1:A:342:TYR:CD2	2.53	0.43
3:C:851:ARG:NH2	3:C:851:ARG:CG	2.81	0.43
1:D:297:TYR:CD2	1:D:321:ASP:HB3	2.54	0.43
1:D:328:PHE:HB2	1:D:351:ILE:HD11	2.01	0.43
1:D:376:ILE:HD13	1:D:424:PRO:HD2	2.01	0.43
3:F:768:GLY:HA2	3:F:794:ILE:CD1	2.49	0.43
3:F:815:LEU:O	3:F:817:ARG:N	2.45	0.43
1:G:395:LYS:C	1:G:397:ILE:N	2.75	0.43
3:I:766:THR:HG22	3:I:767:ILE:N	2.33	0.43
1:D:61:ARG:HH21	1:D:106:GLN:CD	2.27	0.43
1:D:137:TYR:O	1:D:138:ARG:C	2.62	0.43
1:D:209:TYR:HA	1:D:210:PRO:HA	1.84	0.43
1:G:227:LEU:O	1:G:230:SER:HB2	2.18	0.43
1:G:242:ASP:OD1	1:G:244:ILE:N	2.52	0.43
1:G:381:ILE:CD1	1:G:424:PRO:HG3	2.39	0.43
3:I:744:ILE:HB	3:I:766:THR:HB	2.00	0.43
3:I:781:VAL:HG22	3:I:817:ARG:NH1	2.32	0.43
1:A:24:ARG:CD	1:A:39:GLN:HG3	2.49	0.42
1:A:53:LEU:HD22	1:A:54:TYR:H	1.84	0.42
1:A:381:ILE:CD1	1:A:424:PRO:HG3	2.39	0.42
3:C:768:GLY:HA2	3:C:794:ILE:CD1	2.49	0.42
1:D:233:MET:HE3	2:E:1443:MET:CE	2.49	0.42
1:G:164:ILE:HD12	1:G:277:ARG:CZ	2.49	0.42
1:G:421:GLU:CD	1:G:421:GLU:H	2.27	0.42
1:A:135:LYS:HD3	1:A:217:LEU:O	2.19	0.42
1:D:116:ILE:C	1:D:118:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ASP:HA	1:D:124:LYS:HD3	2.01	0.42
1:D:128:LYS:O	1:D:129:LYS:HB2	2.18	0.42
1:D:189:LYS:HA	1:D:189:LYS:HD3	1.82	0.42
1:D:421:GLU:CD	1:D:421:GLU:H	2.27	0.42
2:E:1436:VAL:HG13	2:E:1437:VAL:N	2.33	0.42
1:G:28:SER:HB2	1:G:428:TYR:O	2.20	0.42
1:G:145:LEU:HD13	1:G:151:ILE:HG12	2.01	0.42
1:G:295:TYR:HB3	3:I:846:ILE:HG22	2.01	0.42
1:G:298:THR:HG22	1:G:299:ALA:H	1.85	0.42
1:G:343:VAL:HG11	3:I:834:ARG:CZ	2.50	0.42
1:G:379:ASN:O	1:G:419:THR:HA	2.19	0.42
1:G:395:LYS:O	1:G:397:ILE:N	2.51	0.42
3:I:737:THR:O	3:I:738:LYS:C	2.62	0.42
3:I:839:SER:O	3:I:843:LEU:HB2	2.19	0.42
3:C:783:LEU:O	3:C:785:ASN:N	2.52	0.42
1:D:107:ASP:C	1:D:109:PHE:N	2.75	0.42
1:D:171:ASN:O	1:D:171:ASN:ND2	2.51	0.42
1:D:183:THR:O	1:D:183:THR:HG22	2.20	0.42
1:G:25:TYR:HD2	1:G:425:ASN:ND2	2.12	0.42
3:I:848:TYR:CE2	3:I:852:LEU:HD22	2.53	0.42
1:A:296:ASP:HB2	1:A:297:TYR:CD1	2.54	0.42
1:A:321:ASP:OD1	1:A:323:SER:HB2	2.19	0.42
3:C:744:ILE:HB	3:C:766:THR:HB	2.01	0.42
1:D:93:VAL:HA	1:D:94:PRO:HD3	1.83	0.42
1:D:136:SER:OG	1:D:139:ASP:HA	2.20	0.42
1:D:242:ASP:OD1	1:D:244:ILE:N	2.52	0.42
1:D:343:VAL:O	1:D:343:VAL:CG1	2.67	0.42
3:C:751:ALA:O	3:C:754:THR:HG22	2.20	0.42
3:F:745:PRO:HG2	3:F:750:LEU:HD21	2.02	0.42
1:G:153:MET:HE1	1:G:212:LEU:O	2.20	0.42
3:I:745:PRO:HG2	3:I:750:LEU:HD21	2.02	0.42
1:A:340:ASP:O	1:A:341:ASN:HB2	2.19	0.42
3:C:799:VAL:HB	3:C:823:LEU:HD21	2.01	0.42
1:D:25:TYR:HD2	1:D:425:ASN:HD22	1.68	0.42
1:D:33:THR:HG23	1:D:49:LEU:HG	2.00	0.42
3:F:737:THR:O	3:F:738:LYS:C	2.62	0.42
3:F:742:TYR:O	3:F:767:ILE:HG13	2.20	0.42
1:G:57:LEU:HD11	1:G:106:GLN:CG	2.48	0.42
1:G:228:ASN:C	1:G:230:SER:N	2.77	0.42
1:G:282:GLN:HG2	1:G:342:TYR:HB3	2.02	0.42
3:I:851:ARG:NH2	3:I:851:ARG:CG	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASN:OD1	1:A:219:ASN:C	2.61	0.42
3:C:742:TYR:O	3:C:767:ILE:HG13	2.20	0.42
1:D:224:ASN:O	1:D:225:LEU:C	2.62	0.42
1:D:239:SER:O	1:D:240:THR:C	2.63	0.42
1:G:21:GLN:O	1:G:23:PRO:N	2.53	0.42
1:G:69:PHE:HA	1:G:83:PHE:O	2.19	0.42
1:G:128:LYS:O	1:G:129:LYS:HB2	2.20	0.42
1:G:371:GLY:HA3	1:G:387:MET:HG2	2.02	0.42
1:G:373:LEU:HD23	1:G:384:VAL:HG21	2.02	0.42
3:I:799:VAL:HB	3:I:823:LEU:HD21	2.01	0.42
1:A:164:ILE:HD12	1:A:277:ARG:CZ	2.50	0.42
1:A:190:ASP:OD1	1:A:192:LEU:N	2.48	0.42
1:A:297:TYR:CD2	1:A:321:ASP:HB3	2.55	0.42
1:A:369:GLN:OE1	1:A:450:ILE:HG21	2.20	0.42
3:F:817:ARG:NH2	3:F:818:LYS:HD3	2.33	0.42
1:G:102:ASP:O	1:G:106:GLN:HB2	2.19	0.42
1:G:356:LEU:O	1:G:358:ARG:N	2.52	0.42
1:G:399:GLU:O	1:G:400:SER:HB2	2.20	0.42
1:A:89:PHE:HB3	1:A:91:MET:HE3	2.02	0.42
1:A:170:ASN:HD22	1:A:176:ASP:CG	2.28	0.42
1:A:189:LYS:HD3	1:A:189:LYS:HA	1.83	0.42
1:A:368:GLU:CD	1:A:368:GLU:N	2.64	0.42
1:A:421:GLU:H	1:A:421:GLU:CD	2.27	0.42
1:D:53:LEU:HD22	1:D:54:TYR:H	1.84	0.42
1:D:90:VAL:HG11	1:D:156:ILE:HD13	2.02	0.42
1:G:42:ILE:HD11	1:G:58:ASN:HD22	1.84	0.42
1:G:220:GLU:HB2	1:G:263:TRP:CH2	2.54	0.42
1:D:57:LEU:HD12	1:D:58:ASN:H	1.85	0.42
1:D:291:PRO:HD3	1:D:350:LEU:HD22	2.02	0.42
1:D:395:LYS:HD3	1:D:399:GLU:OE2	2.20	0.42
1:D:420:ILE:HD12	1:D:420:ILE:C	2.45	0.42
1:G:248:ASN:ND2	1:G:342:TYR:CZ	2.84	0.42
1:A:167:ASN:OD1	1:A:178:ARG:HB2	2.19	0.41
1:A:320:ASP:C	1:A:322:GLY:N	2.77	0.41
1:D:164:ILE:CD1	1:D:277:ARG:CZ	2.98	0.41
1:D:336:SER:HB2	1:D:342:TYR:CD2	2.55	0.41
3:C:847:ASN:O	3:C:847:ASN:ND2	2.53	0.41
1:G:250:ILE:O	1:G:254:GLN:HG3	2.20	0.41
1:G:397:ILE:HG12	2:H:1449:ILE:HD12	2.01	0.41
3:I:768:GLY:HA2	3:I:794:ILE:HD12	2.02	0.41
1:A:43:ILE:HG13	1:A:59:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PRO:HD3	1:A:350:LEU:HD22	2.01	0.41
1:A:437:LEU:HB2	1:A:450:ILE:HD11	2.03	0.41
2:B:1434:PHE:CD1	2:B:1435:LYS:N	2.79	0.41
3:C:802:TYR:O	3:C:803:VAL:C	2.63	0.41
3:C:816:ASN:ND2	3:C:816:ASN:O	2.46	0.41
3:F:738:LYS:HB2	3:F:741:TYR:CD2	2.52	0.41
1:G:325:ILE:HD12	1:G:327:LEU:HD21	2.01	0.41
1:A:134:PRO:HD2	1:A:187:PHE:CE1	2.55	0.41
1:A:137:TYR:HA	1:A:217:LEU:HG	2.02	0.41
1:D:226:ILE:CG2	1:D:227:LEU:N	2.83	0.41
3:C:839:SER:O	3:C:843:LEU:HB2	2.20	0.41
1:D:236:SER:O	1:D:237:LEU:C	2.63	0.41
3:F:802:TYR:O	3:F:804:ASP:N	2.52	0.41
2:H:1441:LEU:HD23	2:H:1441:LEU:HA	1.81	0.41
3:I:804:ASP:CG	3:I:805:ASP:H	2.27	0.41
1:A:61:ARG:HH21	1:A:106:GLN:CD	2.29	0.41
1:A:449:ASN:O	1:A:450:ILE:HD13	2.20	0.41
1:D:308:ASP:OD1	1:D:309:ASN:N	2.54	0.41
1:D:417:ILE:HG22	1:D:418:ALA:N	2.35	0.41
1:G:223:LEU:O	1:G:226:ILE:HG22	2.21	0.41
1:G:417:ILE:HG22	1:G:418:ALA:N	2.35	0.41
3:I:797:LYS:C	3:I:823:LEU:HD13	2.46	0.41
3:I:818:LYS:HD2	3:I:818:LYS:N	2.30	0.41
1:A:103:VAL:O	1:A:103:VAL:HG12	2.21	0.41
1:A:325:ILE:HD12	1:A:327:LEU:HD21	2.03	0.41
1:D:93:VAL:HB	1:D:95:TRP:NE1	2.35	0.41
1:D:234:TYR:C	1:D:236:SER:N	2.76	0.41
3:F:802:TYR:O	3:F:803:VAL:C	2.63	0.41
1:G:93:VAL:HB	1:G:95:TRP:HE1	1.85	0.41
1:G:356:LEU:HD21	1:G:414:LEU:HD21	2.03	0.41
1:G:425:ASN:HB3	1:G:440:MET:HB3	2.02	0.41
3:I:755:ASN:HB2	3:I:759:GLU:O	2.21	0.41
1:A:248:ASN:HD21	1:A:339:VAL:HG21	1.85	0.41
1:A:288:ASN:HA	1:A:289:PRO:C	2.46	0.41
1:A:395:LYS:O	1:A:397:ILE:N	2.54	0.41
1:D:369:GLN:OE1	1:D:450:ILE:HG21	2.20	0.41
2:H:1436:VAL:HG13	2:H:1437:VAL:N	2.36	0.41
3:I:751:ALA:O	3:I:754:THR:HG22	2.20	0.41
1:A:119:GLU:O	1:A:124:LYS:NZ	2.53	0.41
1:A:149:ASP:HB2	1:A:178:ARG:NH2	2.36	0.41
1:A:417:ILE:HG22	1:A:418:ALA:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:755:ASN:HB2	3:C:759:GLU:O	2.20	0.41
3:C:802:TYR:O	3:C:804:ASP:N	2.54	0.41
1:D:103:VAL:O	1:D:103:VAL:HG12	2.19	0.41
3:F:742:TYR:CD1	3:F:743:THR:N	2.89	0.41
3:F:818:LYS:HD2	3:F:818:LYS:N	2.31	0.41
1:G:102:ASP:HB3	1:G:105:ILE:HB	2.02	0.41
1:G:320:ASP:C	1:G:322:GLY:N	2.77	0.41
1:G:449:ASN:O	1:G:450:ILE:HD13	2.21	0.41
3:I:802:TYR:O	3:I:803:VAL:C	2.64	0.41
3:C:768:GLY:HA2	3:C:794:ILE:HD12	2.03	0.41
3:C:837:ILE:N	3:C:837:ILE:HD12	2.36	0.41
1:D:35:ILE:O	1:D:45:TRP:HA	2.21	0.41
1:D:79:LEU:HD12	1:D:139:ASP:HB2	2.03	0.41
1:D:102:ASP:HB3	1:D:105:ILE:HB	2.02	0.41
1:D:296:ASP:OD1	3:F:845:ASP:HB3	2.21	0.41
3:F:847:ASN:O	3:F:847:ASN:ND2	2.54	0.41
1:G:43:ILE:HG13	1:G:59:PHE:CE2	2.56	0.41
1:G:194:LEU:HB3	1:G:208:PHE:HB2	2.02	0.41
1:G:336:SER:HB2	1:G:342:TYR:CD2	2.56	0.41
1:G:440:MET:HE2	1:G:440:MET:HB2	1.88	0.41
3:I:738:LYS:HB2	3:I:741:TYR:CD2	2.53	0.41
3:I:843:LEU:HD12	3:I:843:LEU:HA	1.88	0.41
1:A:39:GLN:O	1:A:40:ASP:C	2.64	0.40
1:A:142:ILE:HD11	1:A:156:ILE:HG12	2.03	0.40
1:A:371:GLY:HA3	1:A:387:MET:HG2	2.03	0.40
1:D:156:ILE:C	1:D:157:LEU:HD23	2.46	0.40
1:D:339:VAL:HG11	1:D:342:TYR:CD1	2.56	0.40
1:G:395:LYS:HD3	1:G:399:GLU:OE2	2.20	0.40
1:A:216:LEU:HB2	1:A:272:ILE:HD11	2.03	0.40
1:A:250:ILE:CG2	2:E:1441:LEU:HG	2.51	0.40
3:C:815:LEU:O	3:C:817:ARG:N	2.48	0.40
3:F:744:ILE:HB	3:F:766:THR:HB	2.02	0.40
3:F:834:ARG:HE	3:F:834:ARG:HB3	1.61	0.40
1:G:93:VAL:HA	1:G:94:PRO:HD3	1.83	0.40
1:G:224:ASN:O	1:G:225:LEU:C	2.62	0.40
1:A:198:ASN:OD1	1:A:198:ASN:C	2.64	0.40
3:C:807:GLN:O	3:C:809:PRO:CD	2.70	0.40
1:D:288:ASN:HA	1:D:289:PRO:C	2.46	0.40
3:F:755:ASN:HB2	3:F:759:GLU:O	2.21	0.40
1:G:107:ASP:C	1:G:109:PHE:N	2.77	0.40
1:G:297:TYR:HD2	1:G:320:ASP:HB2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321:ASP:OD1	1:G:323:SER:HB2	2.21	0.40
3:I:742:TYR:CD1	3:I:743:THR:N	2.89	0.40
3:I:762:VAL:HG22	3:I:763:SER:N	2.36	0.40
3:I:813:GLU:O	3:I:814:GLY:C	2.64	0.40
1:A:10:LEU:HG	1:A:11:PRO:CD	2.49	0.40
1:A:174:GLY:HA2	3:C:859:GLN:HE22	1.86	0.40
1:A:206:PHE:CZ	1:A:284:PRO:HG3	2.56	0.40
1:A:422:ARG:HG2	1:A:422:ARG:H	1.72	0.40
1:D:133:HIS:HB3	1:D:136:SER:HB3	2.03	0.40
1:D:194:LEU:HB3	1:D:208:PHE:HB2	2.03	0.40
3:F:751:ALA:O	3:F:754:THR:HG22	2.22	0.40
1:G:121:VAL:CG1	1:G:122:GLY:N	2.83	0.40
1:G:288:ASN:HA	1:G:289:PRO:C	2.45	0.40
1:A:216:LEU:HB2	1:A:272:ILE:HD12	2.04	0.40
1:D:237:LEU:CD2	1:D:246:LYS:HA	2.52	0.40
1:D:310:GLY:O	1:D:312:ASN:N	2.55	0.40
2:E:1432:LYS:HG3	2:E:1433:GLY:H	1.84	0.40
3:F:799:VAL:HB	3:F:823:LEU:HD21	2.03	0.40
1:G:89:PHE:HB3	1:G:91:MET:HE3	2.04	0.40
1:G:137:TYR:CZ	1:G:269:LYS:HD3	2.56	0.40
1:G:418:ALA:HB3	1:G:439:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	449/452 (99%)	358 (80%)	64 (14%)	27 (6%)	1	7
1	D	445/452 (98%)	351 (79%)	65 (15%)	29 (6%)	1	6
1	G	445/452 (98%)	358 (80%)	62 (14%)	25 (6%)	1	9
2	B	26/39 (67%)	21 (81%)	5 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	26/39 (67%)	21 (81%)	4 (15%)	1 (4%)	2	15
2	H	26/39 (67%)	20 (77%)	6 (23%)	0	100	100
3	C	145/152 (95%)	110 (76%)	24 (17%)	11 (8%)	1	5
3	F	145/152 (95%)	110 (76%)	24 (17%)	11 (8%)	1	5
3	I	145/152 (95%)	110 (76%)	24 (17%)	11 (8%)	1	5
All	All	1852/1929 (96%)	1459 (79%)	278 (15%)	115 (6%)	1	7

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	GLU
1	A	266	ARG
1	A	311	GLN
1	A	377	SER
3	C	738	LYS
3	C	784	THR
3	C	803	VAL
1	D	51	ASP
1	D	98	SER
1	D	123	PRO
1	D	139	ASP
1	D	311	GLN
1	D	377	SER
2	E	1432	LYS
3	F	738	LYS
3	F	784	THR
3	F	803	VAL
1	G	311	GLN
1	G	377	SER
3	I	738	LYS
3	I	784	THR
3	I	803	VAL
1	A	4	SER
1	A	48	VAL
1	A	51	ASP
1	A	200	THR
1	A	294	LEU
1	A	308	ASP
3	C	757	LYS
3	C	816	ASN

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Mol	Chain	Res	Type
3	C	849	GLU
1	D	48	VAL
1	D	176	ASP
1	D	200	THR
1	D	240	THR
1	D	266	ARG
1	D	294	LEU
1	D	308	ASP
1	D	321	ASP
3	F	757	LYS
3	F	816	ASN
3	F	849	GLU
1	G	8	SER
1	G	48	VAL
1	G	51	ASP
1	G	120	GLU
1	G	200	THR
1	G	266	ARG
1	G	294	LEU
1	G	308	ASP
1	G	321	ASP
3	I	757	LYS
3	I	816	ASN
3	I	849	GLU
1	A	20	SER
1	A	85	ASP
1	A	137	TYR
1	A	321	ASP
1	A	357	GLN
3	C	814	GLY
1	D	20	SER
1	D	172	SER
1	D	357	GLN
1	D	396	SER
3	F	814	GLY
1	G	20	SER
1	G	85	ASP
1	G	357	GLN
1	G	396	SER
3	I	814	GLY
1	A	8	SER
1	A	22	SER

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Mol	Chain	Res	Type
1	A	29	SER
1	D	22	SER
1	D	29	SER
1	D	85	ASP
1	G	22	SER
1	G	29	SER
1	G	442	ASN
3	I	737	THR
1	A	50	THR
1	A	172	SER
1	A	368	GLU
1	A	442	ASN
1	A	445	LEU
3	C	737	THR
3	C	785	ASN
3	C	806	ASN
1	D	50	THR
1	D	120	GLU
1	D	169	PRO
1	D	368	GLU
1	D	417	ILE
1	D	442	ASN
3	F	737	THR
3	F	785	ASN
3	F	806	ASN
1	G	50	THR
1	G	121	VAL
1	G	368	GLU
1	G	417	ILE
3	I	785	ASN
3	I	806	ASN
1	A	417	ILE
1	G	23	PRO
1	A	11	PRO
3	C	808	LYS
1	D	11	PRO
1	D	23	PRO
1	A	23	PRO
3	F	808	LYS
1	G	11	PRO
1	G	367	PRO
1	A	367	PRO

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Mol	Chain	Res	Type
3	I	808	LYS

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	422/423 (100%)	390 (92%)	32 (8%)	12	38
1	D	418/423 (99%)	387 (93%)	31 (7%)	13	38
1	G	418/423 (99%)	387 (93%)	31 (7%)	13	38
2	B	24/33 (73%)	22 (92%)	2 (8%)	10	35
2	E	24/33 (73%)	23 (96%)	1 (4%)	26	52
2	H	24/33 (73%)	22 (92%)	2 (8%)	10	35
3	C	130/132 (98%)	123 (95%)	7 (5%)	20	47
3	F	130/132 (98%)	123 (95%)	7 (5%)	20	47
3	I	130/132 (98%)	124 (95%)	6 (5%)	24	50
All	All	1720/1764 (98%)	1601 (93%)	119 (7%)	14	40

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	7	LEU
1	A	10	LEU
1	A	21	GLN
1	A	68	THR
1	A	139	ASP
1	A	141	CYS
1	A	142	ILE
1	A	157	LEU
1	A	159	SER
1	A	201	GLU
1	A	210	PRO
1	A	217	LEU

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Mol	Chain	Res	Type
1	A	225	LEU
1	A	242	ASP
1	A	243	VAL
1	A	247	ARG
1	A	249	VAL
1	A	251	LYS
1	A	257	SER
1	A	267	PHE
1	A	277	ARG
1	A	281	VAL
1	A	297	TYR
1	A	352	GLU
1	A	361	LYS
1	A	384	VAL
1	A	386	PHE
1	A	408	LEU
1	A	421	GLU
1	A	431	TRP
1	A	443	LYS
2	B	1432	LYS
2	B	1441	LEU
3	C	816	ASN
3	C	818	LYS
3	C	834	ARG
3	C	841	ASP
3	C	843	LEU
3	C	864	LYS
3	C	875	PHE
1	D	10	LEU
1	D	21	GLN
1	D	68	THR
1	D	98	SER
1	D	139	ASP
1	D	157	LEU
1	D	159	SER
1	D	198	ASN
1	D	201	GLU
1	D	210	PRO
1	D	217	LEU
1	D	225	LEU
1	D	236	SER
1	D	242	ASP

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Mol	Chain	Res	Type
1	D	243	VAL
1	D	247	ARG
1	D	251	LYS
1	D	257	SER
1	D	267	PHE
1	D	277	ARG
1	D	281	VAL
1	D	297	TYR
1	D	352	GLU
1	D	361	LYS
1	D	384	VAL
1	D	386	PHE
1	D	408	LEU
1	D	420	ILE
1	D	421	GLU
1	D	431	TRP
1	D	443	LYS
2	E	1441	LEU
3	F	816	ASN
3	F	818	LYS
3	F	834	ARG
3	F	841	ASP
3	F	843	LEU
3	F	864	LYS
3	F	875	PHE
1	G	10	LEU
1	G	21	GLN
1	G	68	THR
1	G	139	ASP
1	G	157	LEU
1	G	159	SER
1	G	171	ASN
1	G	176	ASP
1	G	198	ASN
1	G	201	GLU
1	G	210	PRO
1	G	217	LEU
1	G	225	LEU
1	G	242	ASP
1	G	243	VAL
1	G	247	ARG
1	G	249	VAL

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Mol	Chain	Res	Type
1	G	251	LYS
1	G	257	SER
1	G	267	PHE
1	G	277	ARG
1	G	281	VAL
1	G	297	TYR
1	G	352	GLU
1	G	361	LYS
1	G	384	VAL
1	G	386	PHE
1	G	408	LEU
1	G	421	GLU
1	G	431	TRP
1	G	443	LYS
2	H	1432	LYS
2	H	1441	LEU
3	I	816	ASN
3	I	818	LYS
3	I	834	ARG
3	I	841	ASP
3	I	843	LEU
3	I	864	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	180	ASN
1	A	273	GLN
1	A	288	ASN
3	C	785	ASN
3	C	793	HIS
3	C	862	GLN
1	D	62	HIS
1	D	113	HIS
1	D	180	ASN
1	D	273	GLN
3	F	785	ASN
3	F	793	HIS
3	F	862	GLN
1	G	113	HIS
1	G	273	GLN

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Mol	Chain	Res	Type
1	G	346	ASN
1	G	436	ASN
3	I	785	ASN
3	I	793	HIS
3	I	862	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	451/452 (99%)	-0.25	1 (0%) 91 87	60, 104, 150, 170	0
1	D	447/452 (98%)	0.03	2 (0%) 88 81	61, 99, 145, 170	0
1	G	447/452 (98%)	-0.23	1 (0%) 91 87	63, 104, 148, 170	0
2	B	28/39 (71%)	-0.41	0 100 100	68, 90, 136, 136	0
2	E	28/39 (71%)	-0.27	0 100 100	65, 87, 127, 136	0
2	H	28/39 (71%)	-0.39	0 100 100	69, 88, 126, 137	0
3	C	147/152 (96%)	-0.14	0 100 100	95, 141, 190, 199	0
3	F	147/152 (96%)	0.06	2 (1%) 73 59	93, 140, 190, 198	0
3	I	147/152 (96%)	0.02	1 (0%) 84 73	96, 141, 190, 199	0
All	All	1870/1929 (96%)	-0.13	7 (0%) 88 81	60, 111, 169, 199	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	378	ASP	3.0
1	D	436	ASN	2.7
1	G	23	PRO	2.5
3	F	762	VAL	2.4
3	F	758	GLY	2.2
1	A	94	PRO	2.1
3	I	752	LYS	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.