



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:45 PM UTC

PDB ID : 2NZ9 / pdb_00002nz9
Title : Crystal structure of botulinum neurotoxin type A complexed with monoclonal antibody AR2
Authors : Stevens, R.C.; Arndt, J.W.
Deposited on : 2006-11-22
Resolution : 3.79 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

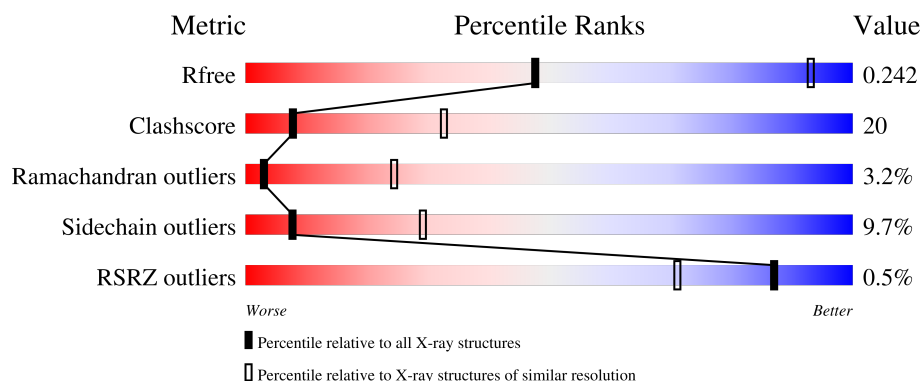
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1295	% 59% 32% 6% ..
1	B	1295	60% 32% 6% ..
2	C	218	% 57% 36% 6% .
2	E	218	% 62% 30% 6% ..
3	D	224	61% 28% 7% ..

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Mol	Chain	Length	Quality of chain
3	F	224	% 63% 29%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26985 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1267	Total	C	N	O	S	0	0	0
			10200	6541	1691	1937	31			
1	B	1267	Total	C	N	O	S	0	0	0
			10203	6543	1691	1938	31			

- Molecule 2 is a protein called AR2 monoclonal antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	216	Total	C	N	O	S	0	0	0
			1657	1039	279	334	5			
2	E	216	Total	C	N	O	S	0	0	0
			1657	1039	279	334	5			

- Molecule 3 is a protein called AR2 monoclonal antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	217	Total	C	N	O	S	0	0	0
			1632	1025	271	329	7			
3	F	217	Total	C	N	O	S	0	0	0
			1632	1025	271	329	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

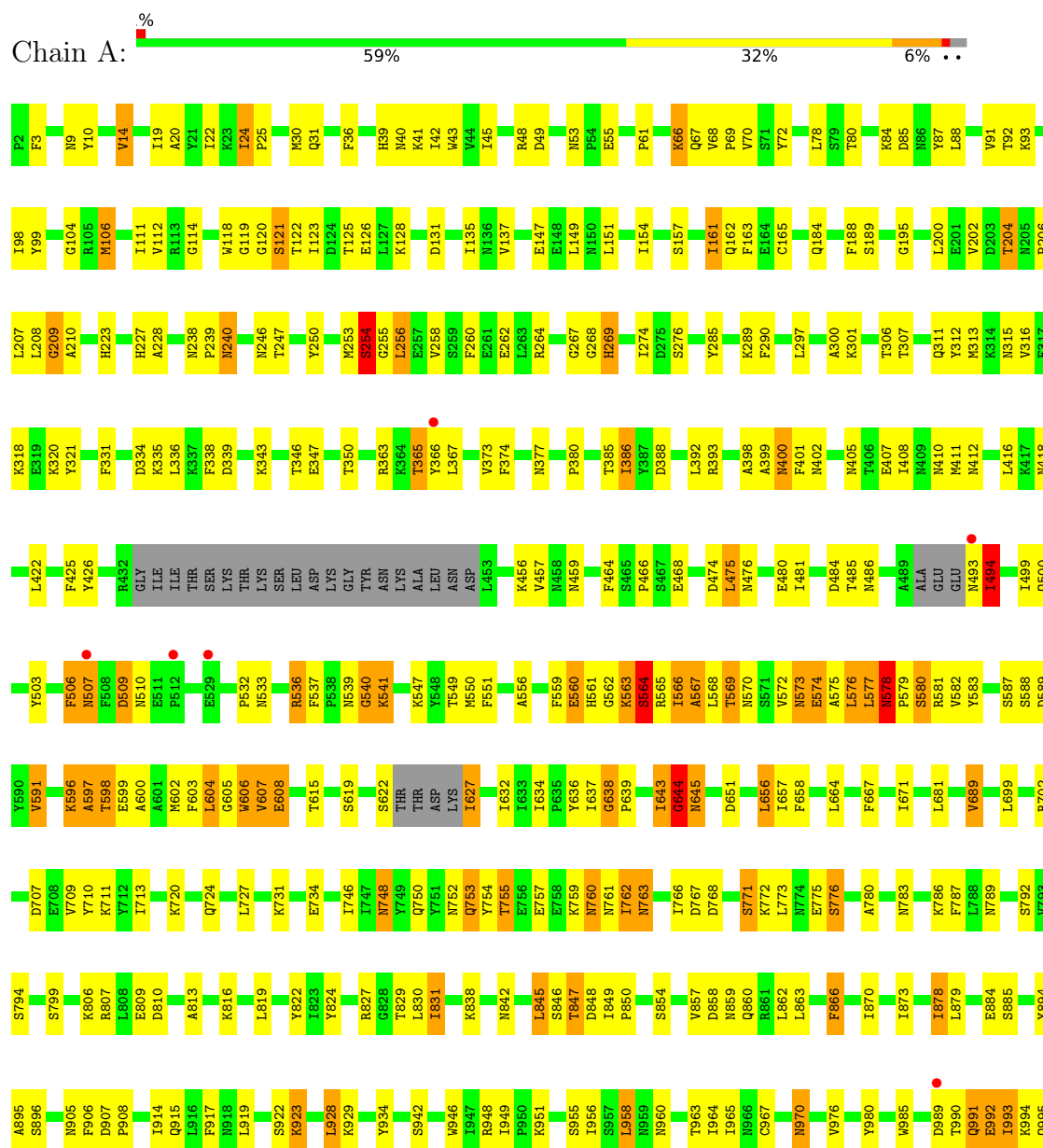
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

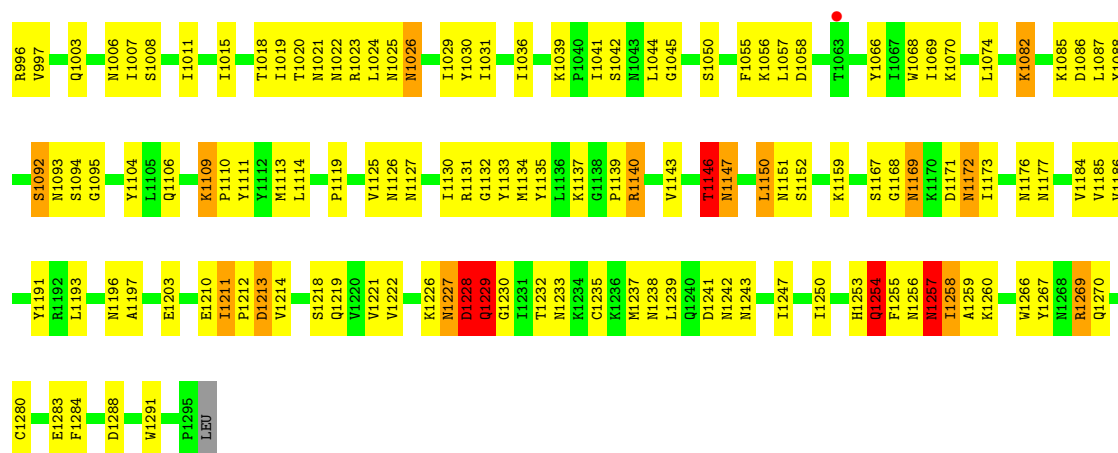
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ca 1	0	0
5	B	1	Total 1	Ca 1	0	0

3 Residue-property plots

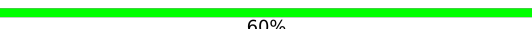
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

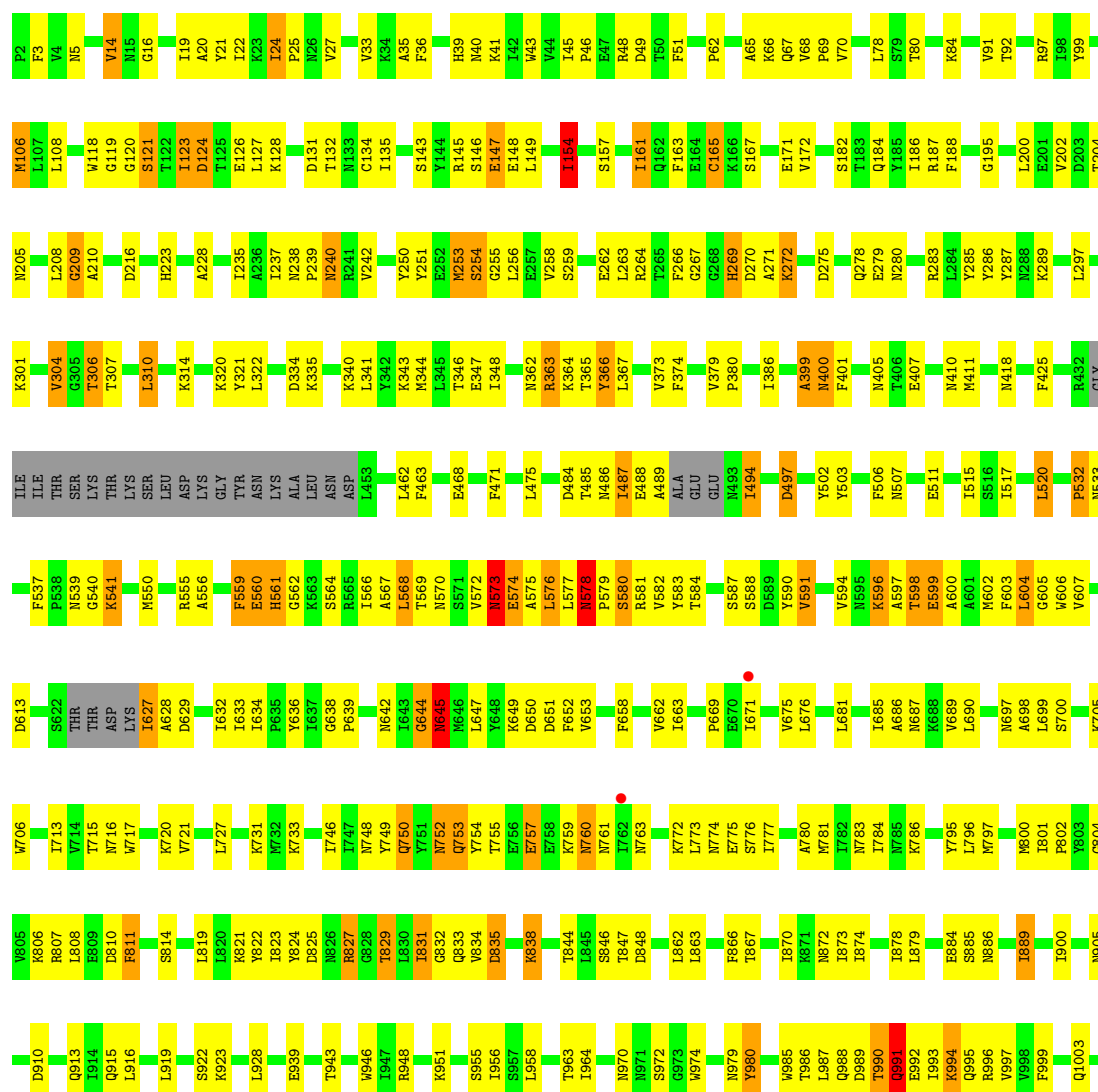
• Molecule 1: Botulinum neurotoxin type A

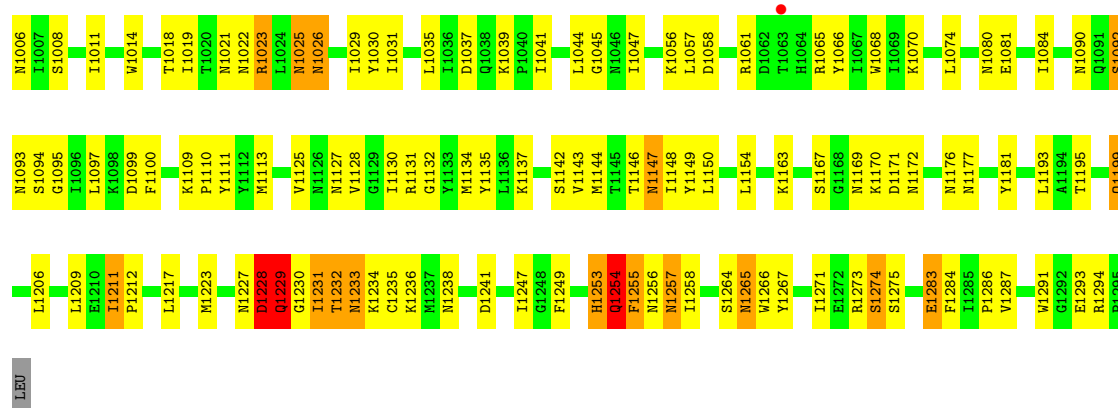




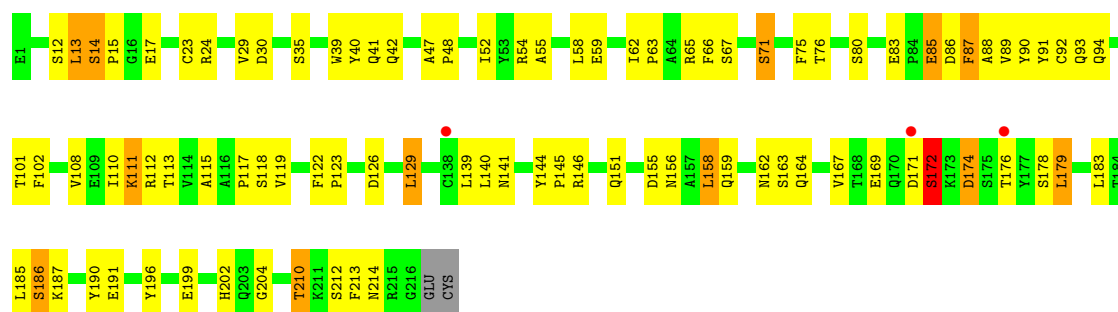
• Molecule 1: Botulinum neurotoxin type A

Chain B:  60%  32%  6% ..

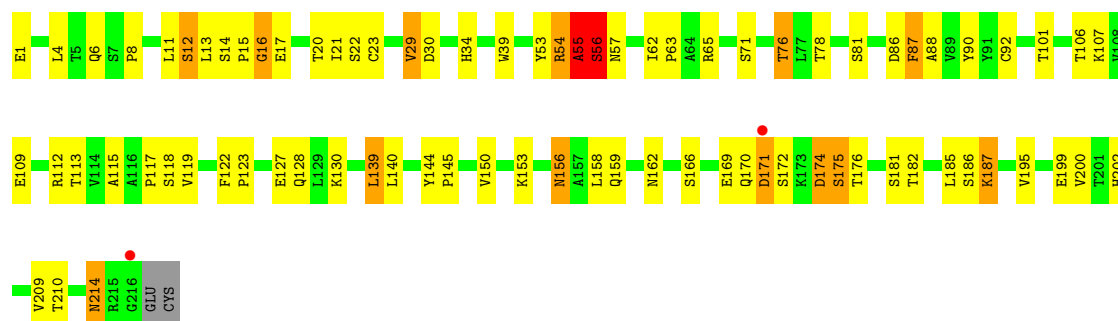




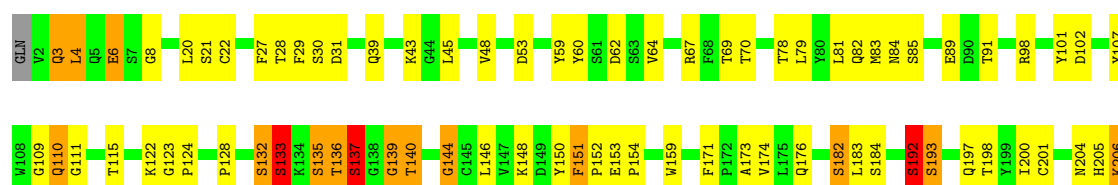
• Molecule 2: AR2 monoclonal antibody

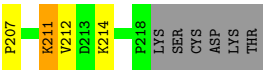


• Molecule 2: AR2 monoclonal antibody

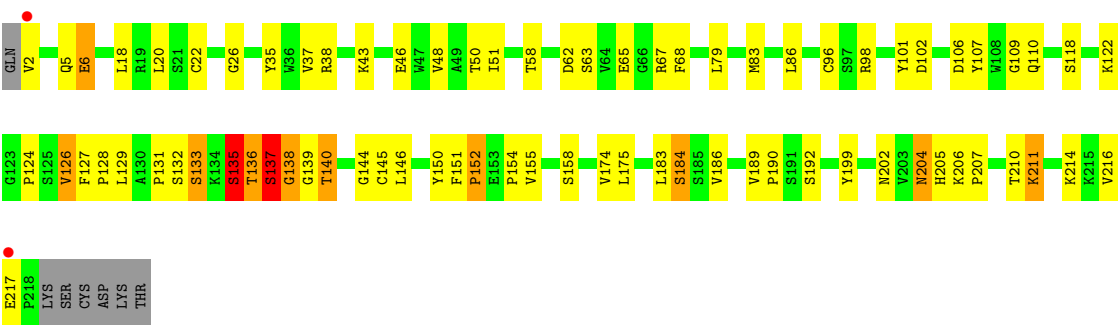


• Molecule 3: AR2 monoclonal antibody





● Molecule 3: AR2 monoclonal antibody



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.97Å 197.60Å 146.10Å 90.00° 91.18° 90.00°	Depositor
Resolution (Å)	40.00 – 3.79 40.00 – 3.79	Depositor EDS
% Data completeness (in resolution range)	95.5 (40.00-3.79) 95.4 (40.00-3.79)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.278 0.203 , 0.242	Depositor DCC
R_{free} test set	2688 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	95.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 127.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	26985	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.72	1/10416 (0.0%)	0.94	14/14098 (0.1%)
1	B	0.72	1/10420 (0.0%)	0.94	11/14104 (0.1%)
2	C	0.71	0/1695	0.90	0/2303
2	E	0.71	0/1695	0.90	0/2303
3	D	0.65	0/1673	0.93	6/2281 (0.3%)
3	F	0.61	0/1673	0.90	1/2281 (0.0%)
All	All	0.71	2/27572 (0.0%)	0.94	32/37370 (0.1%)

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	26
1	B	0	27
2	C	0	3
2	E	0	3
3	D	0	6
3	F	0	5
All	All	0	70

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	960	ASN	C-O	5.81	1.30	1.23
1	B	587	SER	C-O	5.27	1.30	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	153	GLU	C-N-CD	-8.33	102.27	120.60
3	D	144	GLY	N-CA-C	6.66	119.86	110.74
3	D	123	GLY	CA-C-N	6.64	126.40	119.76
3	D	123	GLY	C-N-CA	6.64	126.40	119.76
1	A	638	GLY	CA-C-N	6.38	125.80	118.85
1	A	638	GLY	C-N-CA	6.38	125.80	118.85
1	A	494	ILE	N-CA-C	6.27	115.64	106.55
1	B	304	VAL	N-CA-C	5.93	116.66	108.12
1	B	1025	ASN	N-CA-C	5.92	117.54	108.30
1	B	287	TYR	N-CA-C	-5.91	104.02	111.11
1	B	878	ILE	N-CA-C	-5.87	107.27	112.90
1	B	797	MET	N-CA-C	5.71	117.30	111.14
1	A	949	ILE	N-CA-C	5.64	113.14	107.55
1	A	689	VAL	N-CA-C	5.42	115.63	110.42
1	A	866	PHE	N-CA-C	-5.37	105.08	111.69
1	B	1195	THR	N-CA-C	5.37	116.31	108.14
1	B	240	ASN	N-CA-C	-5.32	106.29	112.89
1	A	878	ILE	N-CA-C	-5.31	107.80	112.90
3	D	3	GLN	N-CA-C	5.29	117.58	109.95
1	A	1109	LYS	CA-C-N	5.26	126.08	119.98
1	A	1109	LYS	C-N-CA	5.26	126.08	119.98
3	D	48	VAL	CB-CA-C	-5.21	105.66	111.80
1	B	1039	LYS	CA-C-N	5.17	125.98	119.98
1	B	1039	LYS	C-N-CA	5.17	125.98	119.98
1	A	61	PRO	CA-C-N	5.15	123.37	119.66
1	A	61	PRO	C-N-CA	5.15	123.37	119.66
1	A	976	VAL	CB-CA-C	-5.14	103.85	110.84
3	F	126	VAL	N-CA-C	5.12	115.42	107.28
1	A	131	ASP	N-CA-C	5.09	116.83	111.28
1	B	1065	ARG	N-CA-C	5.09	117.25	110.53
1	B	154	ILE	CB-CA-C	-5.04	103.98	111.19
1	A	240	ASN	N-CA-C	-5.02	107.10	113.18

There are no chirality outliers.

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1139	PRO	Peptide
1	A	1167	SER	Peptide
1	A	118	TRP	Peptide
1	A	119	GLY	Peptide
1	A	1226	LYS	Peptide
1	A	1227	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	1228	ASP	Peptide
1	A	1232	THR	Peptide
1	A	1254	GLN	Peptide
1	A	1257	ASN	Peptide
1	A	484	ASP	Peptide
1	A	507	ASN	Peptide
1	A	547	LYS	Peptide
1	A	564	SER	Peptide
1	A	573	ASN	Peptide
1	A	574	GLU	Peptide
1	A	578	ASN	Peptide
1	A	596	LYS	Peptide
1	A	598	THR	Peptide
1	A	604	LEU	Peptide
1	A	644	GLY	Peptide
1	A	645	ASN	Peptide
1	A	753	GLN	Peptide
1	A	847	THR	Peptide
1	A	989	ASP	Peptide
1	A	992	GLU	Peptide
1	B	118	TRP	Peptide
1	B	119	GLY	Peptide
1	B	120	GLY	Peptide
1	B	1228	ASP	Peptide
1	B	1229	GLN	Peptide
1	B	1232	THR	Peptide
1	B	1254	GLN	Peptide
1	B	148	GLU	Peptide
1	B	487	ILE	Peptide
1	B	532	PRO	Peptide
1	B	559	PHE	Peptide
1	B	564	SER	Peptide
1	B	573	ASN	Peptide
1	B	574	GLU	Peptide
1	B	578	ASN	Peptide
1	B	596	LYS	Peptide
1	B	604	LEU	Peptide
1	B	644	GLY	Peptide
1	B	645	ASN	Peptide
1	B	649	LYS	Peptide
1	B	650	ASP	Peptide
1	B	753	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	B	847	THR	Peptide
1	B	989	ASP	Peptide
1	B	990	THR	Peptide
1	B	991	GLN	Peptide
1	B	994	LYS	Peptide
2	C	117	PRO	Peptide
2	C	171	ASP	Peptide
2	C	172	SER	Peptide
3	D	133	SER	Peptide
3	D	135	SER	Peptide
3	D	136	THR	Peptide
3	D	137	SER	Peptide
3	D	139	GLY	Peptide
3	D	8	GLY	Peptide
2	E	171	ASP	Peptide
2	E	172	SER	Peptide
2	E	55	ALA	Peptide
3	F	133	SER	Peptide
3	F	135	SER	Peptide
3	F	136	THR	Peptide
3	F	137	SER	Peptide
3	F	152	PRO	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	10200	0	10003	384	0
1	B	10203	0	9999	403	0
2	C	1657	0	1595	66	0
2	E	1657	0	1595	71	0
3	D	1632	0	1552	68	0
3	F	1632	0	1552	74	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	26985	0	26296	1058	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 20.

All (1058) 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:B:269:HIS:CD2	1:B:365:THR:HG21	1.40	1.56
1:A:596:LYS:CB	1:A:597:ALA:HB3	1.39	1.47
3:F:132:SER:HA	3:F:133:SER:CB	1.42	1.46
1:B:540:GLY:CA	1:B:541:LYS:HB2	1.40	1.43
1:B:578:ASN:HB3	1:B:579:PRO:CA	1.41	1.43
1:A:578:ASN:HB3	1:A:579:PRO:C	1.43	1.42
1:B:540:GLY:HA2	1:B:541:LYS:CB	1.44	1.40
3:D:139:GLY:N	3:D:140:THR:HB	1.34	1.38
3:D:132:SER:HA	3:D:133:SER:CB	1.44	1.34
3:D:132:SER:CA	3:D:133:SER:HB3	1.59	1.33
1:B:578:ASN:HB3	1:B:579:PRO:C	1.53	1.32
3:F:132:SER:CA	3:F:133:SER:HB3	1.62	1.29
1:A:596:LYS:HB2	1:A:597:ALA:CB	1.64	1.27
1:A:992:GLU:CA	1:A:993:ILE:HG13	1.63	1.26
1:A:1044:LEU:HB3	1:A:1045:GLY:CA	1.65	1.24
1:A:578:ASN:HB3	1:A:579:PRO:CA	1.62	1.23
1:B:488:GLU:HA	1:B:489:ALA:CB	1.60	1.23
3:F:139:GLY:CA	3:F:140:THR:HB	1.69	1.22
1:B:573:ASN:HA	1:B:575:ALA:H	1.06	1.21
1:A:1044:LEU:CB	1:A:1045:GLY:HA2	1.69	1.21
3:F:139:GLY:HA3	3:F:140:THR:CB	1.72	1.20
3:D:139:GLY:CA	3:D:140:THR:HB	1.70	1.18
3:D:136:THR:HB	3:D:137:SER:CA	1.73	1.17
1:B:532:PRO:HA	1:B:533:ASN:CB	1.74	1.17
1:A:579:PRO:HA	1:A:581:ARG:H	1.09	1.14
2:C:14:SER:O	2:C:17:GLU:HG3	1.42	1.13
1:B:488:GLU:CA	1:B:489:ALA:HB3	1.77	1.13
1:B:269:HIS:CD2	1:B:365:THR:CG2	2.31	1.12
1:B:532:PRO:HA	1:B:533:ASN:HB2	1.15	1.12
1:B:578:ASN:HB3	1:B:579:PRO:HA	1.17	1.12
3:F:136:THR:HB	3:F:137:SER:CA	1.81	1.10
2:E:12:SER:O	2:E:13:LEU:HD12	1.52	1.09
1:A:67:GLN:HA	1:A:425:PHE:CE1	1.88	1.09
1:A:540:GLY:HA2	1:A:541:LYS:HB2	1.13	1.09
1:B:68:VAL:CG2	1:B:69:PRO:HD2	1.84	1.08
2:E:144:TYR:CG	2:E:145:PRO:HA	1.88	1.08
1:B:135:ILE:HG23	1:B:149:LEU:HD22	1.36	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:GLU:CA	1:A:993:ILE:CG1	2.29	1.08
1:B:573:ASN:HA	1:B:575:ALA:N	1.66	1.08
1:B:578:ASN:CB	1:B:579:PRO:CA	2.30	1.06
1:B:578:ASN:CB	1:B:579:PRO:HA	1.85	1.06
1:B:627:ILE:HD12	1:B:628:ALA:H	1.11	1.06
1:B:1228:ASP:HB3	1:B:1229:GLN:CB	1.85	1.05
1:B:1228:ASP:HB3	1:B:1229:GLN:HB3	1.37	1.05
1:A:540:GLY:HA2	1:A:541:LYS:CB	1.89	1.03
1:B:579:PRO:HA	1:B:581:ARG:H	1.18	1.03
1:B:1211:ILE:CG1	1:B:1212:PRO:HD3	1.90	1.02
1:A:532:PRO:HA	1:A:533:ASN:CB	1.88	1.01
1:A:540:GLY:CA	1:A:541:LYS:HB2	1.90	1.01
3:D:139:GLY:CA	3:D:140:THR:CB	2.37	1.00
1:A:209:GLY:HA3	1:A:405:ASN:ND2	1.75	1.00
1:A:596:LYS:CA	1:A:597:ALA:HB3	1.93	0.99
1:A:14:VAL:HG12	1:A:20:ALA:HA	1.42	0.99
1:A:578:ASN:CB	1:A:579:PRO:C	2.34	0.98
1:A:1044:LEU:HB3	1:A:1045:GLY:HA2	1.00	0.97
3:D:136:THR:CB	3:D:137:SER:CA	2.41	0.97
1:B:209:GLY:HA3	1:B:405:ASN:HD21	1.24	0.97
1:B:1044:LEU:HB3	1:B:1045:GLY:HA2	1.47	0.97
1:B:135:ILE:HG23	1:B:149:LEU:CD2	1.94	0.96
1:A:596:LYS:CA	1:A:597:ALA:CB	2.44	0.96
2:E:174:ASP:HB2	2:E:176:THR:HG22	1.44	0.95
1:B:578:ASN:CB	1:B:579:PRO:C	2.39	0.95
1:B:269:HIS:HD2	1:B:365:THR:CG2	1.74	0.95
3:F:204:ASN:ND2	3:F:211:LYS:HG3	1.82	0.95
1:B:364:LYS:O	1:B:365:THR:HG23	1.65	0.94
3:F:136:THR:CB	3:F:137:SER:CA	2.45	0.94
1:B:269:HIS:NE2	1:B:365:THR:HG21	1.84	0.92
1:A:604:LEU:N	1:A:605:GLY:HA3	1.83	0.92
1:A:578:ASN:CB	1:A:579:PRO:CA	2.48	0.91
1:B:67:GLN:HA	1:B:425:PHE:CE1	2.06	0.91
1:B:68:VAL:HG23	1:B:69:PRO:HD2	1.49	0.91
1:A:579:PRO:HA	1:A:581:ARG:N	1.84	0.91
3:D:139:GLY:HA3	3:D:140:THR:CB	1.99	0.90
1:A:532:PRO:HA	1:A:533:ASN:HB2	1.49	0.90
1:A:561:HIS:N	1:A:562:GLY:HA3	1.84	0.90
1:B:1211:ILE:HG13	1:B:1212:PRO:HD3	1.50	0.90
2:E:144:TYR:CD1	2:E:145:PRO:HA	2.06	0.90
1:B:264:ARG:HD2	1:B:346:THR:HB	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:MET:HA	1:A:1113:MET:HE2	1.54	0.89
1:B:270:ASP:OD1	1:B:365:THR:HB	1.71	0.89
1:B:627:ILE:HD12	1:B:628:ALA:N	1.88	0.89
1:A:993:ILE:CG2	1:A:1044:LEU:HD11	2.02	0.88
1:B:532:PRO:CA	1:B:533:ASN:CB	2.49	0.88
3:D:132:SER:HA	3:D:133:SER:HB2	1.53	0.88
1:B:209:GLY:HA3	1:B:405:ASN:ND2	1.88	0.88
3:D:139:GLY:H	3:D:140:THR:CB	1.84	0.88
1:B:269:HIS:HD2	1:B:365:THR:HG21	1.11	0.87
3:D:132:SER:CA	3:D:133:SER:CB	2.31	0.87
1:B:1044:LEU:HB3	1:B:1045:GLY:CA	2.04	0.87
1:B:68:VAL:HG22	1:B:69:PRO:HD2	1.54	0.86
3:F:204:ASN:HD21	3:F:211:LYS:HG3	1.37	0.86
1:B:594:VAL:HA	1:B:606:TRP:HZ2	1.41	0.86
1:B:1113:MET:HE2	1:B:1113:MET:HA	1.56	0.86
3:F:139:GLY:HA3	3:F:140:THR:HB	0.88	0.86
1:B:569:THR:HA	1:B:582:VAL:HG13	1.58	0.85
1:B:1273:ARG:O	1:B:1274:SER:HB2	1.75	0.85
1:B:579:PRO:HA	1:B:581:ARG:N	1.91	0.84
1:A:596:LYS:HA	1:A:597:ALA:CB	2.07	0.84
3:D:132:SER:HA	3:D:133:SER:HB3	0.85	0.84
1:B:364:LYS:O	1:B:365:THR:CG2	2.26	0.84
2:E:119:VAL:HG21	2:E:209:VAL:HG21	1.59	0.84
1:A:578:ASN:HB3	1:A:579:PRO:HA	1.58	0.84
1:B:135:ILE:CG2	1:B:149:LEU:HD22	2.08	0.83
1:B:1228:ASP:C	1:B:1230:GLY:H	1.86	0.83
1:A:264:ARG:HD2	1:A:346:THR:HB	1.60	0.83
1:B:596:LYS:HB2	1:B:597:ALA:HB3	1.58	0.83
1:B:561:HIS:N	1:B:562:GLY:HA2	1.92	0.83
1:B:604:LEU:N	1:B:605:GLY:HA3	1.93	0.83
2:E:54:ARG:HG3	2:E:54:ARG:HH11	1.42	0.82
3:F:98:ARG:NH1	3:F:107:TYR:HD1	1.78	0.82
1:B:488:GLU:HA	1:B:489:ALA:HB3	0.83	0.81
2:C:144:TYR:CD1	2:C:145:PRO:HA	2.15	0.81
2:C:13:LEU:HG	2:C:17:GLU:OE1	1.80	0.81
3:D:135:SER:OG	3:D:136:THR:HA	1.80	0.81
3:F:204:ASN:HD21	3:F:211:LYS:CG	1.94	0.80
1:B:573:ASN:CA	1:B:575:ALA:H	1.90	0.80
1:B:1044:LEU:CB	1:B:1045:GLY:HA2	2.09	0.80
1:A:561:HIS:H	1:A:562:GLY:CA	1.95	0.80
1:B:596:LYS:CA	1:B:597:ALA:HB3	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1228:ASP:CB	1:B:1229:GLN:HB3	2.12	0.80
1:A:532:PRO:CA	1:A:533:ASN:CB	2.59	0.80
1:A:596:LYS:CB	1:A:597:ALA:CB	2.34	0.80
1:B:596:LYS:CB	1:B:597:ALA:HB3	2.11	0.80
1:A:532:PRO:HA	1:A:533:ASN:HB3	1.64	0.80
1:B:238:ASN:HD22	1:B:239:PRO:HD2	1.46	0.80
1:A:385:THR:HG23	1:A:392:LEU:HD21	1.64	0.79
3:D:139:GLY:H	3:D:140:THR:HB	0.99	0.79
1:A:561:HIS:N	1:A:562:GLY:CA	2.46	0.78
1:B:1253:HIS:O	1:B:1254:GLN:HB2	1.82	0.78
1:B:379:VAL:HB	1:B:380:PRO:HD3	1.63	0.78
3:D:139:GLY:HA3	3:D:140:THR:OG1	1.82	0.78
1:A:253:MET:HE1	1:A:256:LEU:HD22	1.66	0.78
1:A:857:VAL:HG12	1:A:859:ASN:H	1.49	0.78
1:A:125:THR:O	1:A:300:ALA:HA	1.84	0.77
1:A:596:LYS:HA	1:A:597:ALA:HB2	1.65	0.77
1:B:1193:LEU:HD11	1:B:1206:LEU:HD13	1.65	0.77
1:A:569:THR:HA	1:A:582:VAL:HG13	1.66	0.76
1:A:121:SER:OG	1:A:126:GLU:CG	2.33	0.76
1:A:532:PRO:CA	1:A:533:ASN:HB3	2.15	0.76
1:B:24:ILE:HG23	1:B:25:PRO:HD2	1.67	0.76
1:B:561:HIS:H	1:B:562:GLY:HA2	1.48	0.76
1:A:992:GLU:CA	1:A:993:ILE:CB	2.63	0.76
1:A:573:ASN:HA	1:A:574:GLU:C	2.12	0.75
1:A:573:ASN:HA	1:A:575:ALA:N	2.00	0.75
3:D:132:SER:CB	3:D:133:SER:HB3	2.16	0.75
1:A:209:GLY:HA3	1:A:405:ASN:HD22	1.49	0.75
1:A:407:GLU:O	1:A:410:ASN:HB3	1.86	0.75
1:A:964:ILE:HG22	1:A:1057:LEU:HD23	1.69	0.75
1:B:1211:ILE:CD1	1:B:1212:PRO:HD3	2.17	0.75
1:A:1126:ASN:OD1	1:A:1127:ASN:N	2.19	0.75
1:B:45:ILE:HB	1:B:154:ILE:HG23	1.68	0.74
1:B:67:GLN:HE22	1:B:537:PHE:H	1.31	0.74
1:B:488:GLU:CA	1:B:489:ALA:CB	2.49	0.74
1:B:1211:ILE:HG13	1:B:1212:PRO:CD	2.17	0.74
3:D:135:SER:HA	3:D:136:THR:O	1.88	0.74
1:A:106:MET:HG2	1:A:506:PHE:CE1	2.23	0.73
1:B:596:LYS:HA	1:B:597:ALA:HB3	1.69	0.73
1:A:121:SER:OG	1:A:126:GLU:HG3	1.87	0.73
1:A:759:LYS:O	1:A:761:ASN:N	2.20	0.73
2:E:54:ARG:O	2:E:55:ALA:HB3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:774:ASN:HA	1:B:777:ILE:HD12	1.71	0.73
1:A:607:VAL:HG12	1:A:608:GLU:N	2.03	0.73
1:B:596:LYS:HA	1:B:597:ALA:CB	2.17	0.73
1:A:767:ASP:O	1:A:771:SER:HB2	1.87	0.73
1:B:40:ASN:HD22	1:B:511:GLU:HG2	1.54	0.73
1:B:559:PHE:HB2	1:B:560:GLU:CA	2.18	0.73
1:A:238:ASN:HD22	1:A:239:PRO:CD	2.02	0.73
1:A:604:LEU:H	1:A:605:GLY:HA3	1.54	0.72
1:A:1113:MET:HE1	1:A:1284:PHE:HA	1.69	0.72
1:A:135:ILE:HG12	1:A:149:LEU:HD22	1.71	0.72
3:D:139:GLY:HA3	3:D:140:THR:HB	1.64	0.72
1:B:1254:GLN:O	1:B:1255:PHE:CD2	2.43	0.72
1:A:568:LEU:N	1:A:580:SER:OG	2.23	0.71
2:E:12:SER:C	2:E:13:LEU:HD12	2.15	0.71
1:A:238:ASN:HD22	1:A:239:PRO:HD2	1.54	0.71
1:A:1221:VAL:HG11	1:A:1237:MET:HB3	1.72	0.71
1:A:1227:ASN:O	1:A:1230:GLY:N	2.23	0.71
1:B:1273:ARG:O	1:B:1274:SER:CB	2.39	0.71
3:F:98:ARG:NH1	3:F:107:TYR:CD1	2.58	0.71
2:E:144:TYR:CG	2:E:145:PRO:CA	2.71	0.71
1:B:238:ASN:ND2	1:B:239:PRO:HD2	2.05	0.71
1:A:757:GLU:O	1:A:760:ASN:N	2.23	0.71
1:A:3:PHE:O	1:A:39:HIS:HD2	1.73	0.70
2:E:16:GLY:HA2	2:E:81:SER:HB2	1.72	0.70
3:D:81:LEU:HG	3:D:83:MET:HE2	1.73	0.70
3:F:132:SER:HA	3:F:133:SER:HB3	0.74	0.70
1:A:575:ALA:O	1:A:576:LEU:C	2.34	0.70
1:A:576:LEU:O	1:A:581:ARG:HB3	1.92	0.70
1:A:1239:LEU:HG	1:A:1247:ILE:HD12	1.72	0.69
1:B:561:HIS:N	1:B:562:GLY:CA	2.56	0.69
1:A:68:VAL:CG2	1:A:69:PRO:HD2	2.21	0.69
1:B:716:ASN:OD1	1:B:720:LYS:HE3	1.92	0.69
2:E:144:TYR:HA	2:E:145:PRO:O	1.92	0.69
1:B:573:ASN:HA	1:B:574:GLU:C	2.17	0.69
2:E:54:ARG:O	2:E:55:ALA:CB	2.41	0.69
3:F:132:SER:HA	3:F:133:SER:HB2	1.63	0.69
1:B:1227:ASN:O	1:B:1229:GLN:C	2.36	0.69
1:B:988:GLN:HG3	1:B:994:LYS:HG3	1.75	0.68
2:E:139:LEU:HD22	3:F:186:VAL:HG21	1.74	0.68
2:C:29:VAL:HG12	2:C:29:VAL:O	1.93	0.68
1:A:573:ASN:CB	1:A:575:ALA:H	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:PRO:HA	1:B:533:ASN:HB3	1.73	0.68
1:B:550:MET:HE3	1:B:731:LYS:HD2	1.75	0.68
2:E:153:LYS:HB3	2:E:156:ASN:HA	1.75	0.68
1:A:754:TYR:O	1:A:755:THR:C	2.37	0.68
1:B:568:LEU:N	1:B:580:SER:OG	2.23	0.68
1:A:634:ILE:HB	1:A:637:ILE:HD12	1.74	0.68
1:A:1211:ILE:CG1	1:A:1212:PRO:HD3	2.24	0.68
1:B:285:TYR:CZ	1:B:289:LYS:HE3	2.29	0.67
1:A:40:ASN:O	1:A:41:LYS:HB2	1.93	0.67
1:B:344:MET:HA	1:B:348:ILE:HD12	1.77	0.67
3:F:132:SER:CA	3:F:133:SER:CB	2.32	0.67
1:A:503:TYR:O	1:A:506:PHE:HB2	1.95	0.67
1:B:627:ILE:CD1	1:B:628:ALA:H	1.97	0.67
3:D:139:GLY:N	3:D:140:THR:CB	2.31	0.66
1:B:1199:GLN:O	1:B:1199:GLN:HG2	1.95	0.66
2:E:8:PRO:O	2:E:106:THR:HG23	1.96	0.66
1:A:67:GLN:HA	1:A:425:PHE:CZ	2.30	0.66
1:B:604:LEU:O	1:B:607:VAL:HB	1.95	0.66
1:A:568:LEU:H	1:A:580:SER:CB	2.09	0.66
1:A:1211:ILE:N	1:A:1212:PRO:HD2	2.11	0.66
1:B:270:ASP:CG	1:B:365:THR:HB	2.21	0.66
1:B:575:ALA:O	1:B:576:LEU:C	2.37	0.66
1:A:70:VAL:HA	1:A:418:ASN:ND2	2.11	0.66
1:B:1023:ARG:HH12	1:B:1047:ILE:H	1.43	0.65
3:D:98:ARG:NH1	3:D:107:TYR:HD1	1.94	0.65
1:B:121:SER:H	1:B:128:LYS:HE2	1.62	0.65
3:F:98:ARG:NH1	3:F:106:ASP:OD1	2.28	0.65
1:B:1211:ILE:HD12	1:B:1212:PRO:HD3	1.78	0.65
1:A:849:ILE:HG23	1:A:850:PRO:HD2	1.77	0.65
1:B:40:ASN:ND2	1:B:511:GLU:HG2	2.11	0.65
1:B:1233:ASN:ND2	1:B:1235:CYS:H	1.94	0.65
2:E:54:ARG:HG3	2:E:54:ARG:NH1	2.11	0.65
1:B:1228:ASP:C	1:B:1230:GLY:N	2.45	0.65
1:A:596:LYS:HB2	1:A:597:ALA:HB3	0.70	0.65
1:B:237:ILE:HG13	1:B:264:ARG:NH2	2.11	0.65
2:E:214:ASN:N	2:E:214:ASN:OD1	2.30	0.65
1:A:163:PHE:CD1	1:A:188:PHE:HA	2.31	0.65
1:B:347:GLU:HB3	1:B:494:ILE:HD11	1.77	0.65
2:E:174:ASP:HB2	2:E:176:THR:CG2	2.24	0.65
1:B:68:VAL:CG2	1:B:69:PRO:CD	2.69	0.64
3:F:51:ILE:HG13	3:F:58:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASN:O	1:B:41:LYS:HB2	1.98	0.64
1:B:806:LYS:NZ	1:B:810:ASP:OD2	2.24	0.64
1:B:1227:ASN:O	1:B:1230:GLY:N	2.30	0.64
2:C:144:TYR:CG	2:C:145:PRO:HA	2.31	0.64
3:F:204:ASN:CG	3:F:211:LYS:HG3	2.22	0.64
1:A:578:ASN:CB	1:A:579:PRO:HA	2.22	0.64
1:A:1203:GLU:OE1	1:A:1253:HIS:HB2	1.97	0.64
1:A:993:ILE:HG22	1:A:1044:LEU:HD21	1.79	0.64
1:A:1150:LEU:O	1:A:1150:LEU:HG	1.97	0.64
1:B:182:SER:O	1:B:184:GLN:NE2	2.30	0.64
1:B:1230:GLY:O	1:B:1231:ILE:C	2.40	0.64
2:E:159:GLN:HG2	2:E:162:ASN:HD21	1.62	0.64
1:B:14:VAL:HG12	1:B:20:ALA:HA	1.78	0.64
2:C:30:ASP:OD1	2:C:35:SER:HA	1.98	0.64
2:C:112:ARG:HH12	2:C:115:ALA:HB2	1.62	0.64
1:A:246:ASN:C	1:A:247:THR:HG23	2.22	0.64
1:A:964:ILE:HA	1:A:1056:LYS:O	1.98	0.64
1:B:365:THR:O	1:B:367:LEU:N	2.31	0.64
1:B:575:ALA:O	1:B:577:LEU:N	2.31	0.64
1:B:1066:TYR:CD1	1:B:1066:TYR:C	2.76	0.64
1:A:10:TYR:N	1:A:85:ASP:OD1	2.27	0.63
1:A:209:GLY:CA	1:A:405:ASN:ND2	2.57	0.63
1:A:1026:ASN:HB3	1:A:1039:LYS:O	1.98	0.63
1:B:596:LYS:CA	1:B:597:ALA:CB	2.75	0.63
1:A:866:PHE:CZ	1:A:870:ILE:HD11	2.33	0.63
1:B:681:LEU:HD11	1:B:819:LEU:HD23	1.81	0.63
3:F:6:GLU:HA	3:F:22:CYS:HA	1.79	0.63
1:A:253:MET:O	1:A:254:SER:C	2.41	0.63
1:B:67:GLN:HE22	1:B:537:PHE:N	1.96	0.63
1:A:1125:VAL:HG22	1:A:1134:MET:HE3	1.80	0.63
3:D:6:GLU:OE1	3:D:111:GLY:N	2.32	0.63
1:B:579:PRO:CA	1:B:581:ARG:H	2.02	0.63
1:A:24:ILE:HG23	1:A:25:PRO:HD2	1.81	0.62
1:A:532:PRO:CB	1:A:533:ASN:HB3	2.29	0.62
3:D:140:THR:HG22	3:D:140:THR:O	1.98	0.62
2:E:112:ARG:NH1	2:E:115:ALA:HB2	2.14	0.62
1:B:1228:ASP:O	1:B:1230:GLY:N	2.30	0.62
1:A:68:VAL:HG22	1:A:69:PRO:HD2	1.81	0.62
1:A:1113:MET:CE	1:A:1284:PHE:HA	2.29	0.62
1:A:1176:ASN:O	1:A:1177:ASN:HB2	1.99	0.62
1:A:388:ASP:OD2	1:A:393:ARG:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASN:OD1	1:B:283:ARG:NH2	2.33	0.62
3:F:124:PRO:HD2	3:F:210:THR:HG21	1.80	0.62
1:B:24:ILE:HG22	1:B:25:PRO:O	2.00	0.62
1:B:68:VAL:HG22	1:B:69:PRO:CD	2.29	0.62
1:A:494:ILE:HG22	1:A:494:ILE:O	2.00	0.62
1:A:578:ASN:HB3	1:A:580:SER:N	2.10	0.61
1:B:343:LYS:HG3	1:B:347:GLU:OE1	1.99	0.61
1:B:993:ILE:CB	1:B:1044:LEU:HD11	2.30	0.61
1:A:1211:ILE:HD12	1:A:1212:PRO:HD3	1.83	0.61
1:B:634:ILE:HD11	1:B:783:ASN:HB3	1.81	0.61
2:E:12:SER:HB2	2:E:109:GLU:HB3	1.80	0.61
3:F:124:PRO:HB3	3:F:150:TYR:HB3	1.82	0.61
1:A:599:GLU:HB2	1:A:600:ALA:HB2	1.82	0.61
1:B:272:LYS:O	1:B:715:THR:HG23	1.99	0.61
1:B:1100:PHE:HD1	1:B:1283:GLU:HG2	1.66	0.61
1:A:120:GLY:O	1:A:121:SER:C	2.43	0.61
1:A:204:THR:O	1:A:206:PRO:HD3	2.00	0.61
1:A:567:ALA:HA	1:A:580:SER:OG	2.00	0.61
2:C:87:PHE:HB3	2:C:110:ILE:HG12	1.82	0.61
2:C:112:ARG:NH1	2:C:115:ALA:HB2	2.16	0.61
1:A:1211:ILE:HG13	1:A:1212:PRO:HD3	1.81	0.61
1:B:578:ASN:HB3	1:B:580:SER:N	2.13	0.61
1:A:1169:ASN:C	1:A:1171:ASP:H	2.08	0.61
1:B:699:LEU:HD22	1:B:844:THR:HG21	1.83	0.61
3:D:204:ASN:ND2	3:D:211:LYS:HG3	2.16	0.61
1:A:993:ILE:HG23	1:A:1044:LEU:HD11	1.83	0.61
1:A:1258:ILE:O	1:A:1260:LYS:N	2.34	0.61
1:B:1008:SER:OG	1:B:1011:ILE:HG13	2.00	0.61
1:A:1211:ILE:N	1:A:1212:PRO:CD	2.63	0.60
1:A:615:THR:O	1:A:619:SER:HB2	2.01	0.60
2:C:202:HIS:CD2	2:C:204:GLY:H	2.19	0.60
3:F:150:TYR:OH	3:F:155:VAL:HG22	2.01	0.60
2:E:20:THR:HG23	2:E:78:THR:HG22	1.84	0.60
3:F:101:TYR:CE2	3:F:102:ASP:HB2	2.36	0.60
1:A:70:VAL:HA	1:A:418:ASN:HD21	1.66	0.60
1:A:985:TRP:HB3	1:A:997:VAL:HG23	1.83	0.60
2:E:140:LEU:HD21	2:E:200:VAL:HG11	1.84	0.60
1:B:757:GLU:O	1:B:760:ASN:N	2.35	0.60
1:B:1241:ASP:HB3	1:B:1247:ILE:HD11	1.83	0.60
2:E:150:VAL:HG11	2:E:181:SER:HB2	1.83	0.60
1:A:806:LYS:HG3	1:A:934:TYR:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:65:ARG:HH21	2:E:86:ASP:CG	2.10	0.59
1:B:823:ILE:CG2	1:B:834:VAL:HG13	2.31	0.59
1:A:1127:ASN:O	1:A:1132:GLY:HA3	2.01	0.59
1:A:993:ILE:HG22	1:A:1044:LEU:HD11	1.81	0.59
1:A:1150:LEU:HD12	1:A:1150:LEU:C	2.28	0.59
1:A:1169:ASN:O	1:A:1171:ASP:N	2.35	0.59
1:A:238:ASN:ND2	1:A:239:PRO:HD2	2.18	0.59
1:B:567:ALA:HB1	1:B:746:ILE:CG1	2.33	0.59
1:B:579:PRO:HB3	1:B:580:SER:HA	1.85	0.59
1:A:627:ILE:HG12	1:A:657:ILE:HG23	1.85	0.58
1:B:301:LYS:O	1:B:310:LEU:HD12	2.03	0.58
1:B:364:LYS:C	1:B:365:THR:HG23	2.28	0.58
1:B:750:GLN:HE21	1:B:750:GLN:HA	1.68	0.58
1:A:859:ASN:OD1	1:A:862:LEU:HD12	2.04	0.58
1:B:532:PRO:CA	1:B:533:ASN:HB3	2.29	0.58
1:B:1113:MET:HE1	1:B:1284:PHE:CD2	2.38	0.58
1:A:604:LEU:N	1:A:605:GLY:CA	2.63	0.58
1:B:559:PHE:CB	1:B:560:GLU:CA	2.81	0.58
1:A:114:GLY:HA2	1:A:320:LYS:HG3	1.85	0.58
1:A:1253:HIS:O	1:A:1254:GLN:HB2	2.03	0.58
1:A:1019:ILE:HD13	1:A:1029:ILE:HG13	1.85	0.58
1:B:579:PRO:CB	1:B:580:SER:HA	2.34	0.58
1:B:1022:ASN:H	1:B:1041:ILE:HD11	1.67	0.58
3:F:205:HIS:CD2	3:F:207:PRO:HD2	2.38	0.58
1:A:634:ILE:HB	1:A:637:ILE:CD1	2.33	0.58
1:A:816:LYS:HB2	1:A:845:LEU:HD23	1.86	0.58
1:A:1119:PRO:O	1:A:1140:ARG:HD2	2.04	0.58
1:B:972:SER:HA	1:B:988:GLN:O	2.02	0.58
3:F:98:ARG:NH1	3:F:106:ASP:CG	2.62	0.58
1:A:121:SER:OG	1:A:126:GLU:HG2	2.03	0.58
1:A:1211:ILE:CD1	1:A:1212:PRO:HD3	2.34	0.58
1:B:1254:GLN:O	1:B:1255:PHE:HD2	1.87	0.58
2:C:159:GLN:HG2	2:C:162:ASN:HD21	1.69	0.58
3:F:20:LEU:HD11	3:F:83:MET:HE1	1.85	0.57
3:F:128:PRO:HB2	3:F:216:VAL:HG13	1.85	0.57
1:A:636:TYR:C	1:A:639:PRO:HD2	2.29	0.57
1:A:1146:THR:O	1:A:1147:ASN:HB2	2.05	0.57
3:F:132:SER:CB	3:F:133:SER:HB3	2.33	0.57
1:A:1104:TYR:HB3	1:A:1173:ILE:HG23	1.85	0.57
2:C:119:VAL:HG22	2:C:140:LEU:HG	1.85	0.57
1:A:643:ILE:HG21	1:A:664:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:PHE:C	1:B:658:PHE:CD2	2.80	0.57
1:A:253:MET:CE	1:A:256:LEU:HD22	2.35	0.57
1:B:532:PRO:CA	1:B:533:ASN:HB2	2.07	0.57
2:E:171:ASP:O	2:E:174:ASP:O	2.23	0.57
1:A:575:ALA:O	1:A:577:LEU:N	2.38	0.57
1:A:1019:ILE:CD1	1:A:1029:ILE:HG13	2.34	0.57
3:F:135:SER:HA	3:F:136:THR:O	2.05	0.57
1:B:946:TRP:HB2	1:B:1070:LYS:HG2	1.87	0.57
1:B:964:ILE:HG22	1:B:1057:LEU:HD23	1.87	0.57
1:B:127:LEU:O	1:B:304:VAL:HG22	2.06	0.56
1:A:195:GLY:HA3	1:A:374:PHE:HE1	1.70	0.56
1:A:709:VAL:O	1:A:713:ILE:HG13	2.05	0.56
2:E:144:TYR:HA	2:E:145:PRO:C	2.29	0.56
1:A:67:GLN:HE22	1:A:537:PHE:N	2.03	0.56
1:A:67:GLN:HE22	1:A:537:PHE:H	1.53	0.56
1:A:658:PHE:C	1:A:658:PHE:CD2	2.83	0.56
1:A:993:ILE:CG2	1:A:1044:LEU:CD1	2.81	0.56
1:A:1257:ASN:C	1:A:1258:ILE:HG12	2.29	0.56
1:B:45:ILE:HB	1:B:154:ILE:CG2	2.35	0.56
1:B:658:PHE:C	1:B:658:PHE:HD2	2.13	0.56
3:D:204:ASN:HD21	3:D:211:LYS:HG3	1.70	0.56
2:E:119:VAL:HG21	2:E:209:VAL:CG2	2.33	0.56
2:E:150:VAL:HG23	2:E:200:VAL:HG22	1.87	0.56
1:A:567:ALA:CA	1:A:580:SER:OG	2.53	0.56
1:B:717:TRP:HH2	1:B:862:LEU:HD13	1.71	0.56
1:B:821:LYS:NZ	1:B:825:ASP:OD2	2.34	0.56
1:A:1113:MET:HE1	1:A:1284:PHE:CD2	2.39	0.56
1:B:205:ASN:HB3	1:B:400:ASN:HB3	1.86	0.56
1:B:238:ASN:OD1	1:B:240:ASN:HB2	2.05	0.56
1:B:310:LEU:HD22	1:B:314:LYS:HG3	1.88	0.56
1:A:951:LYS:HE2	1:A:1151:ASN:OD1	2.05	0.56
1:A:702:ARG:HD2	1:A:845:LEU:HD11	1.88	0.56
1:B:1227:ASN:ND2	1:B:1231:ILE:O	2.39	0.56
2:C:12:SER:O	2:C:13:LEU:HD13	2.06	0.56
1:B:49:ASP:OD1	1:B:49:ASP:C	2.48	0.56
2:C:196:TYR:HB2	2:C:213:PHE:CE1	2.41	0.56
1:A:599:GLU:HB2	1:A:600:ALA:CA	2.36	0.56
3:D:206:LYS:N	3:D:207:PRO:CD	2.69	0.56
1:A:992:GLU:CA	1:A:993:ILE:HB	2.35	0.55
1:B:21:TYR:HA	1:B:33:VAL:O	2.05	0.55
1:A:1113:MET:HE2	1:A:1113:MET:CA	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:974:TRP:HB3	1:B:987:LEU:CD2	2.36	0.55
1:A:578:ASN:C	1:A:581:ARG:HG2	2.31	0.55
1:B:713:ILE:HD11	1:B:804:GLY:HA3	1.87	0.55
1:B:948:ARG:HG3	1:B:1014:TRP:HA	1.88	0.55
3:D:20:LEU:CD1	3:D:83:MET:HE1	2.37	0.55
1:A:573:ASN:HA	1:A:575:ALA:H	1.70	0.55
1:B:167:SER:OG	1:B:184:GLN:NE2	2.38	0.55
1:B:1154:LEU:HD12	1:B:1291:TRP:CE2	2.41	0.55
1:A:468:GLU:OE1	1:A:720:LYS:NZ	2.33	0.55
3:F:150:TYR:CZ	3:F:155:VAL:HG22	2.41	0.55
1:A:209:GLY:HA3	1:A:405:ASN:HD21	1.67	0.55
2:C:54:ARG:O	2:C:55:ALA:HB3	2.07	0.55
1:A:1211:ILE:O	1:A:1214:VAL:HG23	2.07	0.55
1:B:757:GLU:O	1:B:759:LYS:CA	2.55	0.55
1:A:579:PRO:HB3	1:A:580:SER:HA	1.89	0.54
1:A:992:GLU:CA	1:A:993:ILE:CD1	2.84	0.54
1:B:24:ILE:HG23	1:B:25:PRO:CD	2.34	0.54
1:B:184:GLN:HG3	1:B:228:ALA:HA	1.88	0.54
1:B:1234:LYS:O	1:B:1236:LYS:HG2	2.07	0.54
2:C:199:GLU:HG3	2:C:210:THR:HG22	1.88	0.54
3:F:154:PRO:O	3:F:205:HIS:HD2	1.89	0.54
1:B:195:GLY:HA3	1:B:374:PHE:HE1	1.71	0.54
1:B:347:GLU:HB3	1:B:494:ILE:CD1	2.37	0.54
3:D:151:PHE:C	3:D:151:PHE:CD2	2.86	0.54
1:A:699:LEU:O	1:A:702:ARG:HB3	2.06	0.54
1:A:824:TYR:O	1:A:827:ARG:HB3	2.08	0.54
1:B:14:VAL:HA	1:B:19:ILE:O	2.07	0.54
1:B:97:ARG:HA	1:B:386:ILE:HG23	1.89	0.54
1:B:570:ASN:O	1:B:583:TYR:HA	2.08	0.54
1:A:560:GLU:N	1:A:561:HIS:CA	2.71	0.54
1:B:135:ILE:CG2	1:B:149:LEU:CD2	2.76	0.54
1:B:1135:TYR:HE1	1:B:1137:LYS:HB3	1.73	0.54
2:C:39:TRP:CZ3	2:C:92:CYS:HB3	2.42	0.54
1:A:573:ASN:CA	1:A:575:ALA:H	2.21	0.54
1:B:322:LEU:HD12	1:B:341:LEU:HB2	1.88	0.54
2:C:83:GLU:HB2	2:C:85:GLU:HG2	1.88	0.54
3:F:35:TYR:CE1	3:F:50:THR:HG23	2.43	0.54
3:F:37:VAL:HG13	3:F:46:GLU:O	2.08	0.54
1:A:905:ASN:HB3	1:A:915:GLN:HB3	1.89	0.54
2:C:202:HIS:HD2	2:C:204:GLY:H	1.56	0.54
2:C:140:LEU:HD12	2:C:140:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:101:TYR:CD2	3:F:102:ASP:HB2	2.43	0.53
1:B:539:ASN:O	1:B:540:GLY:C	2.51	0.53
1:A:809:GLU:HB3	1:A:934:TYR:CD1	2.44	0.53
1:A:946:TRP:HB2	1:A:1070:LYS:HG2	1.89	0.53
1:A:965:ILE:HG12	1:A:1055:PHE:CD2	2.44	0.53
1:B:146:SER:CB	1:B:520:LEU:HD22	2.38	0.53
1:B:638:GLY:HA3	1:B:652:PHE:HB2	1.91	0.53
1:B:1061:ARG:HG2	1:B:1061:ARG:HH11	1.72	0.53
2:C:159:GLN:CG	2:C:162:ASN:HD21	2.21	0.53
3:D:6:GLU:HA	3:D:22:CYS:HA	1.91	0.53
2:E:139:LEU:CD2	3:F:186:VAL:HG21	2.39	0.53
3:D:200:ILE:HG22	3:D:201:CYS:H	1.74	0.53
1:A:573:ASN:HB3	1:A:575:ALA:H	1.72	0.53
1:B:596:LYS:O	1:B:598:THR:HG22	2.09	0.53
2:E:34:HIS:CD2	2:E:54:ARG:HE	2.27	0.53
1:B:1169:ASN:C	1:B:1171:ASP:H	2.16	0.53
1:B:463:PHE:CD2	1:B:727:LEU:HD23	2.44	0.53
1:B:1018:THR:HG21	1:B:1084:ILE:HG12	1.91	0.53
2:E:140:LEU:HD21	2:E:200:VAL:CG1	2.39	0.53
1:A:599:GLU:HB2	1:A:600:ALA:CB	2.38	0.53
3:F:2:VAL:HG13	3:F:26:GLY:O	2.09	0.53
1:B:485:THR:HG22	1:B:486:ASN:N	2.24	0.53
2:E:54:ARG:HB2	2:E:57:ASN:OD1	2.09	0.53
2:E:144:TYR:CD2	2:E:145:PRO:CA	2.92	0.53
3:F:131:PRO:O	3:F:133:SER:HB2	2.08	0.53
3:F:189:VAL:HB	3:F:190:PRO:CD	2.39	0.53
3:F:129:LEU:HD21	3:F:146:LEU:HB2	1.91	0.53
1:A:894:TYR:O	1:A:929:LYS:HG3	2.09	0.52
1:B:811:PHE:C	1:B:811:PHE:CD2	2.87	0.52
1:B:567:ALA:HB1	1:B:746:ILE:HG12	1.91	0.52
1:B:1008:SER:CB	1:B:1011:ILE:HG13	2.39	0.52
3:F:189:VAL:HB	3:F:190:PRO:HD2	1.92	0.52
1:A:605:GLY:O	1:A:606:TRP:C	2.53	0.52
1:A:1211:ILE:HG13	1:A:1212:PRO:CD	2.39	0.52
1:B:1211:ILE:N	1:B:1212:PRO:CD	2.71	0.52
1:A:1133:TYR:CD1	1:A:1260:LYS:HG2	2.45	0.52
1:A:632:ILE:O	1:A:787:PHE:HD1	1.93	0.52
1:B:885:SER:O	1:B:886:ASN:HB2	2.09	0.52
1:B:1125:VAL:HG22	1:B:1134:MET:HE3	1.90	0.52
1:A:72:TYR:CE1	1:A:416:LEU:HD13	2.44	0.52
1:A:80:THR:O	1:A:84:LYS:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LEU:O	1:A:578:ASN:N	2.42	0.52
3:F:189:VAL:HG11	3:F:199:TYR:CE2	2.44	0.52
2:E:186:SER:O	2:E:187:LYS:C	2.52	0.52
1:A:267:GLY:HA3	1:A:350:THR:HB	1.92	0.52
3:F:126:VAL:HG12	3:F:214:LYS:HG2	1.92	0.52
1:A:838:LYS:O	1:A:842:ASN:HB2	2.09	0.52
1:A:985:TRP:HB3	1:A:997:VAL:CG2	2.39	0.52
1:B:574:GLU:OE1	1:B:574:GLU:N	2.42	0.52
1:A:48:ARG:HG2	1:A:78:LEU:HD23	1.92	0.51
1:A:426:TYR:CE1	1:A:456:LYS:HG2	2.46	0.51
1:A:579:PRO:CB	1:A:580:SER:HA	2.40	0.51
1:A:759:LYS:C	1:A:761:ASN:N	2.68	0.51
1:A:963:THR:HB	1:A:1058:ASP:HB3	1.92	0.51
1:B:146:SER:OG	1:B:520:LEU:HD22	2.10	0.51
2:E:55:ALA:HB3	2:E:56:SER:HB3	1.91	0.51
2:E:65:ARG:NH2	2:E:86:ASP:OD1	2.38	0.51
1:A:1266:TRP:CH2	1:A:1270:GLN:HG3	2.44	0.51
1:A:377:ASN:OD1	1:A:380:PRO:HD3	2.11	0.51
1:A:859:ASN:O	1:A:863:LEU:HG	2.11	0.51
1:A:990:THR:O	1:A:991:GLN:CB	2.59	0.51
1:B:46:PRO:O	1:B:84:LYS:HD3	2.10	0.51
3:F:6:GLU:OE2	3:F:96:CYS:N	2.38	0.51
3:F:98:ARG:HH11	3:F:107:TYR:HD1	1.56	0.51
1:A:3:PHE:HB2	1:A:99:TYR:CD2	2.45	0.51
1:A:550:MET:HE3	1:A:731:LYS:HD2	1.92	0.51
1:A:854:SER:HA	1:A:863:LEU:HD22	1.92	0.51
1:A:934:TYR:N	1:A:934:TYR:CD2	2.78	0.51
1:A:1228:ASP:O	1:A:1229:GLN:C	2.52	0.51
1:B:379:VAL:CB	1:B:380:PRO:HD3	2.35	0.51
1:B:1061:ARG:HG2	1:B:1061:ARG:NH1	2.25	0.51
2:E:199:GLU:HB2	2:E:210:THR:HG22	1.93	0.51
1:A:710:TYR:O	1:A:711:LYS:C	2.54	0.51
1:A:759:LYS:C	1:A:761:ASN:H	2.14	0.51
1:B:1254:GLN:NE2	1:B:1255:PHE:HA	2.25	0.51
1:B:99:TYR:HB2	1:B:108:LEU:CD1	2.40	0.51
1:B:990:THR:O	1:B:991:GLN:CB	2.59	0.51
1:B:1080:ASN:O	1:B:1081:GLU:C	2.53	0.51
1:B:1227:ASN:O	1:B:1227:ASN:CG	2.53	0.51
1:A:188:PHE:CG	1:A:189:SER:N	2.79	0.51
1:A:464:PHE:CD2	1:A:466:PRO:HD3	2.46	0.51
1:A:993:ILE:HG22	1:A:993:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:963:THR:HB	1:B:1058:ASP:HB3	1.93	0.51
2:C:183:LEU:HD21	2:C:185:LEU:HD11	1.92	0.51
1:A:599:GLU:HB2	1:A:600:ALA:HA	1.92	0.51
1:B:242:VAL:HG12	1:B:259:SER:HA	1.93	0.51
1:B:636:TYR:C	1:B:639:PRO:HD2	2.36	0.51
1:B:1099:ASP:C	1:B:1099:ASP:OD1	2.53	0.51
2:E:144:TYR:CD2	2:E:145:PRO:HA	2.40	0.51
1:A:68:VAL:HG13	1:A:68:VAL:O	2.11	0.51
1:B:1113:MET:HE1	1:B:1284:PHE:CG	2.46	0.51
1:B:1211:ILE:CB	1:B:1212:PRO:HD3	2.37	0.51
1:A:125:THR:O	1:A:301:LYS:N	2.37	0.50
1:A:636:TYR:O	1:A:639:PRO:HD2	2.12	0.50
2:C:155:ASP:O	2:C:156:ASN:ND2	2.44	0.50
1:A:634:ILE:HD11	1:A:783:ASN:HB3	1.93	0.50
1:A:1254:GLN:HG2	1:A:1256:ASN:H	1.76	0.50
1:B:1127:ASN:O	1:B:1132:GLY:HA3	2.11	0.50
3:D:146:LEU:HD21	3:D:148:LYS:HD3	1.93	0.50
1:A:72:TYR:CZ	1:A:416:LEU:HD13	2.46	0.50
1:A:238:ASN:ND2	1:A:240:ASN:H	2.09	0.50
1:B:67:GLN:HA	1:B:425:PHE:CZ	2.47	0.50
1:A:1241:ASP:C	1:A:1243:ASN:H	2.19	0.50
1:A:1257:ASN:O	1:A:1258:ILE:HG12	2.12	0.50
1:B:1233:ASN:ND2	1:B:1235:CYS:N	2.60	0.50
2:E:62:ILE:HG23	2:E:63:PRO:HD2	1.94	0.50
3:F:135:SER:CB	3:F:136:THR:HA	2.41	0.50
1:A:464:PHE:CE2	1:A:466:PRO:HD3	2.46	0.50
1:A:923:LYS:O	1:A:923:LYS:HG3	2.12	0.50
1:A:1159:LYS:HB2	1:A:1185:VAL:HB	1.94	0.50
1:B:80:THR:O	1:B:84:LYS:HG3	2.11	0.50
1:B:487:ILE:HD12	1:B:700:SER:HB2	1.94	0.50
1:B:780:ALA:O	1:B:783:ASN:HB2	2.12	0.50
1:B:997:VAL:HB	1:B:1037:ASP:HB3	1.93	0.50
2:E:87:PHE:CD1	2:E:87:PHE:C	2.90	0.50
1:A:607:VAL:O	1:A:608:GLU:C	2.54	0.50
1:A:1044:LEU:CG	1:A:1045:GLY:HA2	2.40	0.50
1:B:267:GLY:HA2	1:B:271:ALA:HB2	1.93	0.50
3:D:84:ASN:O	3:D:85:SER:C	2.54	0.50
1:A:313:MET:O	1:A:316:VAL:HB	2.11	0.50
1:A:1210:GLU:C	1:A:1212:PRO:HD2	2.36	0.50
1:B:49:ASP:OD2	1:B:187:ARG:NE	2.35	0.50
1:B:1273:ARG:O	1:B:1273:ARG:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:98:ARG:NH1	3:D:107:TYR:CD1	2.79	0.50
1:A:120:GLY:O	1:A:121:SER:O	2.30	0.50
1:A:246:ASN:C	1:A:247:THR:CG2	2.85	0.50
1:B:16:GLY:O	1:B:145:ARG:NH2	2.45	0.50
1:B:594:VAL:HA	1:B:606:TRP:CZ2	2.32	0.50
1:B:995:GLN:HB3	1:B:1041:ILE:HG22	1.94	0.50
1:A:42:ILE:HG12	1:A:151:LEU:HB3	1.94	0.49
1:B:831:ILE:HG23	1:B:832:GLY:N	2.26	0.49
1:A:135:ILE:CG1	1:A:149:LEU:HD22	2.41	0.49
1:A:955:SER:HA	1:A:958:LEU:HD12	1.94	0.49
1:B:22:ILE:HG12	1:B:35:ALA:HB3	1.93	0.49
2:E:39:TRP:CZ3	2:E:92:CYS:HB3	2.47	0.49
1:B:1169:ASN:O	1:B:1171:ASP:N	2.39	0.49
3:D:176:GLN:CD	3:D:182:SER:HB3	2.38	0.49
2:E:174:ASP:C	2:E:176:THR:H	2.20	0.49
1:A:559:PHE:HB2	1:A:560:GLU:CA	2.42	0.49
1:B:463:PHE:CE2	1:B:727:LEU:HD23	2.47	0.49
1:B:1111:TYR:CD2	1:B:1284:PHE:HB3	2.47	0.49
1:B:1229:GLN:HG2	1:B:1229:GLN:O	2.12	0.49
2:C:29:VAL:O	2:C:29:VAL:CG1	2.60	0.49
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.46	0.49
1:A:1026:ASN:CB	1:A:1039:LYS:O	2.60	0.49
1:B:399:ALA:O	1:B:401:PHE:N	2.46	0.49
1:B:681:LEU:CD1	1:B:819:LEU:HD23	2.42	0.49
2:C:83:GLU:CB	2:C:85:GLU:HG2	2.42	0.49
1:A:334:ASP:O	1:A:335:LYS:C	2.55	0.49
1:A:819:LEU:O	1:A:822:TYR:HB3	2.13	0.49
1:B:485:THR:CG2	1:B:486:ASN:N	2.76	0.49
1:B:669:PRO:HG3	1:B:721:VAL:CG2	2.42	0.49
1:B:939:GLU:HB3	1:B:1023:ARG:HB2	1.94	0.49
1:A:1169:ASN:C	1:A:1171:ASP:N	2.70	0.49
1:B:216:ASP:OD1	1:B:216:ASP:C	2.55	0.49
1:B:555:ARG:HD3	1:B:581:ARG:HH12	1.76	0.49
2:E:15:PRO:C	2:E:17:GLU:H	2.21	0.49
3:F:68:PHE:CZ	3:F:83:MET:HG2	2.47	0.49
1:B:1238:ASN:HB2	1:B:1249:PHE:CE2	2.48	0.49
1:B:1249:PHE:HB2	1:B:1267:TYR:HB2	1.95	0.49
3:F:101:TYR:HA	3:F:102:ASP:HA	1.50	0.49
1:B:578:ASN:CG	1:B:579:PRO:C	2.80	0.49
1:B:590:TYR:O	1:B:594:VAL:HG22	2.13	0.49
1:B:717:TRP:CD1	1:B:796:LEU:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:150:VAL:HG13	2:E:150:VAL:O	2.12	0.49
3:F:206:LYS:N	3:F:207:PRO:CD	2.76	0.49
1:A:878:ILE:HD11	1:A:1074:LEU:HG	1.95	0.49
1:B:1264:SER:C	1:B:1266:TRP:H	2.20	0.49
2:C:39:TRP:CH2	2:C:92:CYS:HB3	2.47	0.49
3:F:137:SER:C	3:F:138:GLY:O	2.55	0.49
1:A:1113:MET:HE1	1:A:1284:PHE:CG	2.49	0.48
1:B:596:LYS:NZ	1:B:598:THR:HB	2.28	0.48
2:C:71:SER:HA	2:C:75:PHE:CE2	2.48	0.48
1:A:68:VAL:HG23	1:A:69:PRO:HD2	1.92	0.48
1:A:561:HIS:H	1:A:562:GLY:HA2	1.75	0.48
1:B:733:LYS:HB2	1:B:781:MET:HE2	1.95	0.48
1:A:1150:LEU:O	1:A:1150:LEU:CG	2.61	0.48
1:B:905:ASN:HB3	1:B:915:GLN:HB3	1.96	0.48
1:B:1113:MET:HE1	1:B:1284:PHE:HA	1.96	0.48
3:D:205:HIS:CD2	3:D:207:PRO:HD2	2.48	0.48
1:B:781:MET:HA	1:B:784:ILE:HD12	1.95	0.48
1:B:1257:ASN:CG	1:B:1258:ILE:H	2.21	0.48
2:E:12:SER:HB2	2:E:109:GLU:OE1	2.12	0.48
3:F:150:TYR:CZ	3:F:155:VAL:CG2	2.96	0.48
3:F:205:HIS:HB3	3:F:210:THR:HB	1.95	0.48
1:A:607:VAL:HG12	1:A:608:GLU:H	1.76	0.48
1:A:786:LYS:O	1:A:789:ASN:HB2	2.13	0.48
1:B:568:LEU:H	1:B:580:SER:CB	2.22	0.48
2:C:88:ALA:HB3	2:C:90:TYR:CE1	2.48	0.48
2:E:21:ILE:HG22	2:E:22:SER:N	2.27	0.48
1:B:910:ASP:O	1:B:913:GLN:HG3	2.13	0.48
1:A:250:TYR:CD1	1:A:250:TYR:C	2.91	0.48
1:B:306:THR:OG1	1:B:307:THR:N	2.44	0.48
1:A:254:SER:HB2	1:A:459:ASN:CG	2.39	0.48
1:A:599:GLU:OE2	1:A:599:GLU:N	2.46	0.48
1:B:49:ASP:O	1:B:49:ASP:CG	2.57	0.48
1:B:502:TYR:O	1:B:503:TYR:C	2.56	0.48
2:E:4:LEU:HD13	2:E:23:CYS:SG	2.53	0.48
1:A:494:ILE:O	1:A:494:ILE:CG2	2.61	0.48
1:A:556:ALA:HB1	1:A:583:TYR:HB3	1.95	0.48
1:A:884:GLU:O	1:A:885:SER:C	2.56	0.48
1:A:1022:ASN:H	1:A:1041:ILE:HD11	1.78	0.48
1:B:379:VAL:N	1:B:380:PRO:CD	2.76	0.48
2:C:54:ARG:HG3	2:C:54:ARG:HH11	1.78	0.48
1:A:53:ASN:ND2	1:A:55:GLU:H	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:VAL:CG1	2:E:29:VAL:O	2.61	0.48
1:A:3:PHE:O	1:A:39:HIS:CD2	2.62	0.47
1:A:588:SER:HA	1:A:591:VAL:HG13	1.96	0.47
1:A:906:PHE:CE2	1:A:914:ILE:HG12	2.48	0.47
1:B:955:SER:O	1:B:958:LEU:HD12	2.14	0.47
2:C:129:LEU:HD21	2:C:190:TYR:CD2	2.49	0.47
2:C:179:LEU:HA	3:D:171:PHE:HE2	1.79	0.47
1:A:563:LYS:O	1:A:565:ARG:N	2.47	0.47
1:A:1257:ASN:N	1:A:1257:ASN:OD1	2.48	0.47
1:B:253:MET:O	1:B:254:SER:C	2.56	0.47
1:B:365:THR:C	1:B:367:LEU:N	2.70	0.47
1:B:1022:ASN:ND2	1:B:1025:ASN:OD1	2.47	0.47
3:F:139:GLY:N	3:F:140:THR:HB	2.24	0.47
1:A:315:ASN:ND2	1:A:318:LYS:HD3	2.28	0.47
1:A:1006:ASN:H	1:A:1006:ASN:ND2	2.10	0.47
1:B:1228:ASP:HB3	1:B:1229:GLN:HB2	1.90	0.47
2:C:172:SER:O	2:C:172:SER:OG	2.30	0.47
1:A:163:PHE:HD1	1:A:188:PHE:HA	1.77	0.47
1:A:1135:TYR:CE1	1:A:1137:LYS:HB3	2.49	0.47
1:B:1233:ASN:HD21	1:B:1235:CYS:HB2	1.79	0.47
1:A:385:THR:HG23	1:A:392:LEU:CD2	2.42	0.47
1:A:563:LYS:O	1:A:564:SER:C	2.58	0.47
1:A:1007:ILE:HD13	1:A:1114:LEU:HD21	1.95	0.47
1:A:1111:TYR:CG	1:A:1284:PHE:HB3	2.49	0.47
1:B:62:PRO:HG2	1:B:65:ALA:HA	1.96	0.47
1:B:362:ASN:ND2	1:B:363:ARG:O	2.46	0.47
1:B:556:ALA:HB2	1:B:576:LEU:CD1	2.45	0.47
1:B:588:SER:HA	1:B:591:VAL:HG22	1.97	0.47
1:B:772:LYS:O	1:B:775:GLU:HB2	2.15	0.47
2:E:128:GLN:HA	3:F:127:PHE:CE2	2.50	0.47
1:B:195:GLY:CA	1:B:374:PHE:HE1	2.28	0.47
1:B:578:ASN:HB2	1:B:581:ARG:N	2.29	0.47
1:B:1113:MET:CE	1:B:1284:PHE:HA	2.45	0.47
3:D:6:GLU:O	3:D:6:GLU:HG2	2.14	0.47
3:D:53:ASP:OD1	3:D:53:ASP:N	2.48	0.47
3:D:101:TYR:CE2	3:D:102:ASP:HB2	2.49	0.47
3:F:98:ARG:HH12	3:F:106:ASP:CG	2.21	0.47
1:A:22:ILE:HG22	1:A:137:VAL:HA	1.96	0.47
1:A:223:HIS:CE1	1:A:262:GLU:OE2	2.66	0.47
1:A:238:ASN:ND2	1:A:239:PRO:CD	2.73	0.47
1:A:1022:ASN:HB3	1:A:1025:ASN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:TRP:CD1	1:B:149:LEU:HD13	2.50	0.47
1:B:471:PHE:CE1	1:B:720:LYS:HE2	2.49	0.47
2:C:59:GLU:HB3	2:C:62:ILE:HG13	1.95	0.47
2:C:167:VAL:HG22	2:C:179:LEU:HD12	1.96	0.47
3:D:183:LEU:HD12	3:D:183:LEU:C	2.40	0.47
1:B:131:ASP:OD1	1:B:132:THR:HG23	2.14	0.47
1:B:995:GLN:OE1	1:B:996:ARG:N	2.46	0.47
1:B:1003:GLN:HA	1:B:1011:ILE:HD11	1.96	0.47
1:A:536:ARG:HE	1:A:536:ARG:HB3	1.54	0.47
1:A:1093:ASN:O	1:A:1095:GLY:N	2.48	0.47
1:B:165:CYS:SG	1:B:186:ILE:HG12	2.54	0.47
1:B:208:LEU:O	1:B:209:GLY:O	2.32	0.47
1:B:644:GLY:H	1:B:645:ASN:CA	2.28	0.47
1:A:1082:LYS:HE3	1:A:1086:ASP:OD2	2.16	0.47
1:B:1264:SER:C	1:B:1266:TRP:N	2.72	0.47
1:A:43:TRP:CD1	1:A:149:LEU:HD13	2.50	0.46
3:D:200:ILE:HG22	3:D:201:CYS:N	2.30	0.46
2:E:150:VAL:HG11	2:E:181:SER:CB	2.44	0.46
1:A:318:LYS:HB2	1:A:331:PHE:CE1	2.50	0.46
1:A:1066:TYR:CD1	1:A:1066:TYR:C	2.93	0.46
1:B:520:LEU:HD22	1:B:520:LEU:H	1.80	0.46
1:B:676:LEU:HD22	1:B:705:LYS:HE3	1.97	0.46
2:C:87:PHE:CD1	2:C:87:PHE:C	2.92	0.46
2:C:213:PHE:CD1	2:C:213:PHE:C	2.94	0.46
1:A:1113:MET:HE1	1:A:1284:PHE:CA	2.44	0.46
1:A:1031:ILE:HG12	1:A:1036:ILE:HG13	1.98	0.46
1:B:596:LYS:HZ3	1:B:598:THR:HB	1.80	0.46
1:A:499:ILE:O	1:A:500:GLN:C	2.57	0.46
1:A:573:ASN:CA	1:A:575:ALA:N	2.74	0.46
1:A:1196:ASN:HD22	1:A:1197:ALA:N	2.14	0.46
2:E:23:CYS:HB2	2:E:39:TRP:CH2	2.50	0.46
1:B:598:THR:O	1:B:754:TYR:OH	2.33	0.46
1:B:754:TYR:O	1:B:755:THR:C	2.59	0.46
2:C:62:ILE:CG2	2:C:63:PRO:HD2	2.45	0.46
2:C:87:PHE:HB3	2:C:110:ILE:CG1	2.46	0.46
3:D:6:GLU:OE1	3:D:109:GLY:C	2.58	0.46
3:D:20:LEU:HG	3:D:83:MET:HE1	1.96	0.46
2:E:144:TYR:CD2	2:E:144:TYR:C	2.93	0.46
1:A:567:ALA:HB1	1:A:746:ILE:HG12	1.97	0.46
1:A:816:LYS:CB	1:A:845:LEU:HD23	2.46	0.46
1:B:131:ASP:OD1	1:B:132:THR:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:THR:C	1:B:367:LEU:H	2.24	0.46
1:B:687:ASN:ND2	1:B:690:LEU:HD13	2.30	0.46
2:E:6:GLN:NE2	2:E:90:TYR:O	2.40	0.46
1:A:400:ASN:C	1:A:402:ASN:N	2.74	0.46
1:B:468:GLU:OE1	1:B:720:LYS:NZ	2.49	0.46
2:C:163:SER:HB3	2:C:183:LEU:HA	1.97	0.46
3:D:4:LEU:HD21	3:D:27:PHE:CZ	2.51	0.46
1:A:93:LYS:HG3	1:A:386:ILE:HG13	1.98	0.46
1:B:22:ILE:HD11	1:B:45:ILE:HD11	1.98	0.46
1:B:573:ASN:HB2	1:B:576:LEU:HD13	1.97	0.46
1:B:1254:GLN:HG2	1:B:1256:ASN:H	1.81	0.46
3:D:144:GLY:HA2	3:D:159:TRP:HH2	1.82	0.46
1:A:98:ILE:O	1:A:104:GLY:HA3	2.16	0.45
1:A:879:LEU:HD12	1:A:879:LEU:HA	1.80	0.45
1:A:948:ARG:NH2	1:A:1288:ASP:OD2	2.49	0.45
1:B:266:PHE:C	1:B:266:PHE:CD2	2.93	0.45
2:C:186:SER:O	2:C:187:LYS:C	2.59	0.45
1:A:24:ILE:HG23	1:A:25:PRO:CD	2.45	0.45
1:B:488:GLU:HG2	1:B:489:ALA:HB3	1.98	0.45
1:B:915:GLN:HB2	1:B:1068:TRP:CZ3	2.51	0.45
2:E:144:TYR:CD2	2:E:145:PRO:N	2.84	0.45
1:B:974:TRP:HB3	1:B:987:LEU:HD23	1.98	0.45
2:C:23:CYS:HB2	2:C:39:TRP:CH2	2.52	0.45
2:C:93:GLN:HB2	2:C:102:PHE:CD2	2.52	0.45
2:C:140:LEU:N	2:C:140:LEU:CD1	2.79	0.45
1:A:227:HIS:CE1	1:A:262:GLU:OE1	2.69	0.45
1:A:1092:SER:O	1:A:1093:ASN:HB2	2.15	0.45
1:A:1211:ILE:HG13	1:A:1211:ILE:H	1.53	0.45
1:B:48:ARG:HG2	1:B:78:LEU:HD23	1.99	0.45
1:B:407:GLU:O	1:B:410:ASN:HB3	2.16	0.45
1:B:532:PRO:CB	1:B:533:ASN:HB3	2.46	0.45
1:A:772:LYS:O	1:A:775:GLU:HB2	2.17	0.45
1:A:907:ASP:HB2	1:A:1068:TRP:CZ3	2.51	0.45
1:A:1126:ASN:CG	1:A:1127:ASN:N	2.75	0.45
2:C:42:GLN:HE22	3:D:39:GLN:HE22	1.65	0.45
1:B:3:PHE:O	1:B:39:HIS:HD2	1.99	0.45
3:D:78:THR:HG22	3:D:79:LEU:N	2.31	0.45
3:D:197:GLN:NE2	3:D:198:THR:O	2.48	0.45
1:B:638:GLY:O	1:B:642:ASN:N	2.49	0.45
2:C:62:ILE:HG22	2:C:66:PHE:HD1	1.82	0.45
3:F:183:LEU:C	3:F:183:LEU:HD12	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ASN:HA	1:A:85:ASP:OD1	2.17	0.45
1:A:599:GLU:CB	1:A:600:ALA:CA	2.93	0.45
1:A:1029:ILE:HG23	1:A:1029:ILE:O	2.17	0.45
1:B:993:ILE:CB	1:B:1044:LEU:CD1	2.94	0.45
1:A:474:ASP:C	1:A:476:ASN:N	2.74	0.45
1:A:780:ALA:O	1:A:783:ASN:HB2	2.16	0.45
1:A:1222:VAL:N	1:A:1238:ASN:O	2.46	0.45
1:A:1253:HIS:O	1:A:1254:GLN:CB	2.64	0.45
1:B:134:CYS:HB3	1:B:147:GLU:O	2.17	0.45
1:B:645:ASN:O	1:B:647:LEU:N	2.49	0.45
3:D:29:PHE:C	3:D:31:ASP:H	2.25	0.45
3:D:192:SER:HB3	3:D:193:SER:H	1.64	0.45
1:A:942:SER:OG	1:A:1020:THR:HA	2.17	0.45
1:A:1086:ASP:O	1:A:1087:LEU:C	2.60	0.45
1:B:757:GLU:C	1:B:759:LYS:CA	2.90	0.45
1:A:457:VAL:HG21	1:A:551:PHE:HB3	1.99	0.44
1:A:762:ILE:O	1:A:763:ASN:C	2.60	0.44
1:B:255:GLY:HA3	1:B:537:PHE:CG	2.52	0.44
1:B:1146:THR:O	1:B:1147:ASN:HB2	2.16	0.44
2:C:54:ARG:HG3	2:C:54:ARG:NH1	2.32	0.44
2:C:91:TYR:CD1	3:D:45:LEU:HD12	2.52	0.44
3:F:204:ASN:HD21	3:F:211:LYS:HG2	1.79	0.44
1:B:1142:SER:HB3	1:B:1150:LEU:HD11	2.00	0.44
1:B:1209:LEU:CD2	1:B:1217:LEU:HD13	2.46	0.44
2:E:21:ILE:HG22	2:E:22:SER:H	1.81	0.44
2:E:87:PHE:O	2:E:88:ALA:HB2	2.18	0.44
1:A:285:TYR:CZ	1:A:289:LYS:HE2	2.53	0.44
2:C:62:ILE:HG22	2:C:63:PRO:HD2	1.98	0.44
1:A:474:ASP:O	1:A:476:ASN:N	2.50	0.44
1:A:1267:TYR:O	1:A:1270:GLN:N	2.51	0.44
1:B:43:TRP:CD1	1:B:149:LEU:CD1	3.00	0.44
3:D:20:LEU:HD12	3:D:83:MET:HE1	1.99	0.44
3:F:35:TYR:CE1	3:F:50:THR:CG2	3.00	0.44
1:A:91:VAL:O	1:A:92:THR:C	2.60	0.44
1:A:207:LEU:HD12	1:A:207:LEU:HA	1.88	0.44
1:B:161:ILE:H	1:B:161:ILE:HG12	1.62	0.44
1:B:686:ALA:HA	1:B:829:THR:HG23	1.99	0.44
1:B:1018:THR:HB	1:B:1030:TYR:HB2	1.99	0.44
2:E:117:PRO:HD3	2:E:202:HIS:CD2	2.52	0.44
1:A:267:GLY:O	1:A:268:GLY:C	2.60	0.44
1:B:752:ASN:C	1:B:754:TYR:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1144:MET:HB3	1:B:1150:LEU:HD13	1.98	0.44
1:B:1284:PHE:O	1:B:1286:PRO:HD3	2.18	0.44
3:F:144:GLY:O	3:F:216:VAL:HG21	2.18	0.44
1:B:1026:ASN:HA	1:B:1041:ILE:HG12	2.00	0.44
2:C:122:PHE:HA	2:C:123:PRO:HD2	1.68	0.44
3:F:38:ARG:HG2	3:F:48:VAL:CG2	2.48	0.44
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	2.00	0.44
1:B:334:ASP:C	1:B:334:ASP:OD1	2.60	0.44
1:B:948:ARG:HG3	1:B:1014:TRP:CA	2.48	0.44
2:C:93:GLN:HE21	2:C:94:GLN:C	2.26	0.44
2:E:127:GLU:HA	2:E:130:LYS:HE3	2.00	0.44
1:A:393:ARG:HA	1:A:398:ALA:HB2	2.00	0.43
1:B:70:VAL:HG13	1:B:418:ASN:CG	2.43	0.43
1:B:146:SER:HB3	1:B:520:LEU:CD2	2.48	0.43
1:B:364:LYS:C	1:B:365:THR:CG2	2.91	0.43
1:B:599:GLU:HA	1:B:600:ALA:HA	1.72	0.43
1:B:1019:ILE:CD1	1:B:1029:ILE:HG13	2.48	0.43
1:B:1022:ASN:HB3	1:B:1025:ASN:HB2	2.00	0.43
1:B:1113:MET:HA	1:B:1113:MET:CE	2.39	0.43
2:C:118:SER:O	2:C:141:ASN:N	2.45	0.43
2:C:174:ASP:O	2:C:176:THR:N	2.43	0.43
2:E:122:PHE:HA	2:E:123:PRO:HD3	1.78	0.43
2:E:170:GLN:NE2	2:E:175:SER:HB3	2.33	0.43
1:A:14:VAL:HA	1:A:19:ILE:O	2.18	0.43
1:A:320:LYS:HD3	1:A:321:TYR:CE1	2.53	0.43
1:B:1176:ASN:O	1:B:1177:ASN:HB2	2.18	0.43
1:A:87:TYR:O	1:A:91:VAL:HG23	2.19	0.43
1:A:338:PHE:O	1:A:339:ASP:C	2.61	0.43
1:A:727:LEU:O	1:A:731:LYS:HG3	2.18	0.43
1:B:251:TYR:O	1:B:462:LEU:HB3	2.18	0.43
1:B:636:TYR:O	1:B:639:PRO:HD2	2.18	0.43
1:B:834:VAL:O	1:B:835:ASP:C	2.62	0.43
1:B:1233:ASN:HD21	1:B:1235:CYS:H	1.64	0.43
2:C:14:SER:O	2:C:17:GLU:CG	2.36	0.43
3:D:135:SER:HA	3:D:136:THR:C	2.43	0.43
1:A:66:LYS:HE3	1:A:162:GLN:NE2	2.34	0.43
1:A:260:PHE:HE2	1:A:274:ILE:HG23	1.83	0.43
1:A:1026:ASN:HB3	1:A:1039:LYS:C	2.44	0.43
1:A:1085:LYS:O	1:A:1088:TYR:HB3	2.18	0.43
2:C:41:GLN:HB2	2:C:90:TYR:CE2	2.54	0.43
3:D:124:PRO:HB3	3:D:150:TYR:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:ARG:NH1	2:E:54:ARG:CG	2.77	0.43
3:F:128:PRO:HA	3:F:216:VAL:HG22	2.00	0.43
1:A:485:THR:CG2	1:A:486:ASN:N	2.82	0.43
1:A:539:ASN:O	1:A:540:GLY:C	2.62	0.43
1:B:862:LEU:O	1:B:863:LEU:C	2.60	0.43
3:F:158:SER:OG	3:F:202:ASN:HB2	2.19	0.43
1:A:576:LEU:C	1:A:581:ARG:HB3	2.43	0.43
1:A:1109:LYS:HA	1:A:1110:PRO:HD3	1.78	0.43
1:A:1168:GLY:O	1:A:1169:ASN:O	2.37	0.43
1:B:974:TRP:HB3	1:B:987:LEU:HD21	2.01	0.43
2:C:156:ASN:O	2:C:156:ASN:CG	2.61	0.43
3:F:136:THR:OG1	3:F:137:SER:CA	2.66	0.43
1:A:36:PHE:CD1	1:A:36:PHE:N	2.87	0.43
1:A:560:GLU:H	1:A:561:HIS:CA	2.32	0.43
1:B:223:HIS:CE1	1:B:262:GLU:OE2	2.71	0.43
1:B:568:LEU:O	1:B:580:SER:HB3	2.19	0.43
1:B:1093:ASN:C	1:B:1095:GLY:H	2.27	0.43
1:A:365:THR:OG1	1:A:367:LEU:HB2	2.18	0.43
1:A:773:LEU:HA	1:A:776:SER:HB2	2.01	0.43
1:B:573:ASN:CB	1:B:576:LEU:HD13	2.49	0.43
1:B:575:ALA:O	1:B:581:ARG:HB3	2.19	0.43
1:B:916:LEU:O	1:B:1066:TYR:HB2	2.18	0.43
1:A:1228:ASP:HB3	1:A:1229:GLN:H	1.65	0.43
1:B:632:ILE:HG13	1:B:786:LYS:HD3	2.01	0.43
1:B:634:ILE:CD1	1:B:783:ASN:HB3	2.49	0.43
1:B:1228:ASP:HB3	1:B:1229:GLN:CA	2.32	0.43
2:E:8:PRO:HG3	2:E:11:LEU:HD13	2.01	0.43
2:E:76:THR:O	2:E:76:THR:CG2	2.66	0.43
3:F:98:ARG:NH1	3:F:106:ASP:OD2	2.51	0.43
1:A:106:MET:SD	1:A:503:TYR:HA	2.59	0.43
1:A:895:ALA:HA	1:A:928:LEU:HD12	2.00	0.43
3:D:151:PHE:HA	3:D:152:PRO:HA	1.83	0.43
1:A:638:GLY:N	1:A:639:PRO:CD	2.82	0.42
1:B:195:GLY:HA3	1:B:374:PHE:CE1	2.53	0.42
1:B:697:ASN:O	1:B:698:ALA:C	2.62	0.42
2:C:111:LYS:O	2:C:112:ARG:HB3	2.18	0.42
3:D:6:GLU:OE1	3:D:110:GLN:N	2.52	0.42
1:A:643:ILE:HA	1:A:644:GLY:HA3	1.76	0.42
1:A:754:TYR:HB3	1:A:755:THR:H	1.59	0.42
1:A:857:VAL:HG12	1:A:858:ASP:N	2.33	0.42
1:B:629:ASP:N	1:B:629:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:PHE:CD1	1:B:1031:ILE:HG13	2.54	0.42
1:B:1113:MET:HE2	1:B:1113:MET:CA	2.39	0.42
1:A:1106:GLN:HA	1:A:1172:ASN:O	2.19	0.42
1:A:1134:MET:HE1	1:A:1184:VAL:HG11	2.00	0.42
1:B:979:ASN:O	1:B:980:TYR:C	2.62	0.42
1:B:1163:LYS:HB2	1:B:1181:TYR:HB2	2.01	0.42
2:E:170:GLN:HG2	2:E:175:SER:O	2.19	0.42
3:F:140:THR:HA	3:F:189:VAL:O	2.19	0.42
1:A:365:THR:C	1:A:367:LEU:N	2.74	0.42
1:A:1057:LEU:HD11	1:A:1066:TYR:HA	2.02	0.42
1:A:1196:ASN:HD22	1:A:1196:ASN:C	2.26	0.42
3:D:128:PRO:HD3	3:D:214:LYS:HE2	1.99	0.42
1:A:907:ASP:OD1	1:A:907:ASP:C	2.62	0.42
1:A:1018:THR:HB	1:A:1030:TYR:HB2	2.02	0.42
1:B:824:TYR:O	1:B:827:ARG:HB3	2.19	0.42
2:C:86:ASP:O	2:C:108:VAL:HG11	2.19	0.42
2:E:112:ARG:HH11	2:E:115:ALA:HB2	1.84	0.42
1:A:311:GLN:O	1:A:312:TYR:C	2.62	0.42
1:B:951:LYS:HD3	1:B:1149:TYR:CG	2.54	0.42
1:B:1265:ASN:HD22	1:B:1265:ASN:HA	1.66	0.42
2:C:47:ALA:O	2:C:48:PRO:C	2.61	0.42
3:F:155:VAL:HG23	3:F:183:LEU:HD21	2.02	0.42
1:A:366:TYR:OH	1:A:464:PHE:CE1	2.72	0.42
1:A:603:PHE:CD2	1:A:603:PHE:O	2.72	0.42
1:A:1193:LEU:HD21	1:A:1250:ILE:HD13	2.01	0.42
1:B:1030:TYR:CE2	1:B:1035:LEU:HD13	2.55	0.42
1:B:1238:ASN:HA	1:B:1249:PHE:HA	2.01	0.42
3:F:18:LEU:O	3:F:83:MET:HB2	2.19	0.42
1:A:658:PHE:C	1:A:658:PHE:HD2	2.24	0.42
1:B:263:LEU:HA	1:B:263:LEU:HD23	1.77	0.42
1:B:484:ASP:O	1:B:485:THR:C	2.63	0.42
1:B:627:ILE:CD1	1:B:628:ALA:N	2.69	0.42
1:B:819:LEU:O	1:B:822:TYR:HB3	2.20	0.42
1:B:879:LEU:HA	1:B:879:LEU:HD12	1.83	0.42
1:B:884:GLU:CG	1:B:889:ILE:HD11	2.49	0.42
3:D:151:PHE:C	3:D:151:PHE:HD2	2.28	0.42
1:A:255:GLY:O	1:A:256:LEU:HB2	2.19	0.42
1:A:967:CYS:SG	1:A:1050:SER:HB3	2.59	0.42
1:A:995:GLN:CG	1:A:996:ARG:H	2.33	0.42
1:A:1146:THR:O	1:A:1147:ASN:CB	2.66	0.42
1:B:250:TYR:C	1:B:250:TYR:CD1	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:MET:N	1:B:802:PRO:HD2	2.34	0.42
2:E:12:SER:C	2:E:13:LEU:CD1	2.89	0.42
3:F:145:CYS:O	3:F:184:SER:HA	2.19	0.42
1:A:184:GLN:HG3	1:A:228:ALA:HA	2.02	0.42
1:A:809:GLU:CB	1:A:934:TYR:CD1	3.03	0.42
1:A:995:GLN:HG3	1:A:996:ARG:H	1.84	0.42
1:A:1008:SER:CB	1:A:1011:ILE:HG13	2.50	0.42
1:A:1186:VAL:HB	1:A:1191:TYR:CE1	2.55	0.42
1:B:106:MET:HG2	1:B:506:PHE:CE1	2.54	0.42
1:B:795:TYR:O	1:B:796:LEU:C	2.63	0.42
1:B:1109:LYS:HA	1:B:1110:PRO:HD3	1.90	0.42
2:C:164:GLN:HE22	3:D:176:GLN:HA	1.85	0.42
3:D:101:TYR:CD2	3:D:102:ASP:HB2	2.55	0.42
3:D:204:ASN:HD21	3:D:211:LYS:CG	2.33	0.42
1:A:907:ASP:HA	1:A:908:PRO:HD3	1.81	0.41
1:B:278:GLN:O	1:B:279:GLU:C	2.62	0.41
2:C:40:TYR:N	2:C:91:TYR:O	2.43	0.41
2:C:42:GLN:HE22	3:D:39:GLN:NE2	2.18	0.41
3:D:59:TYR:CD1	3:D:59:TYR:N	2.88	0.41
2:E:53:TYR:CE1	2:E:57:ASN:HB2	2.54	0.41
1:A:10:TYR:CZ	1:A:84:LYS:HD2	2.55	0.41
1:B:633:ILE:HG21	1:B:653:VAL:HG22	2.01	0.41
1:B:1254:GLN:HE21	1:B:1255:PHE:C	2.27	0.41
1:B:1291:TRP:CD1	1:B:1293:GLU:HB3	2.55	0.41
1:A:343:LYS:HG3	1:A:347:GLU:OE1	2.21	0.41
1:A:830:LEU:O	1:A:831:ILE:C	2.63	0.41
1:B:91:VAL:O	1:B:92:THR:C	2.63	0.41
2:E:30:ASP:HA	2:E:34:HIS:O	2.20	0.41
2:E:65:ARG:HD2	2:E:81:SER:O	2.21	0.41
3:F:6:GLU:OE1	3:F:109:GLY:HA3	2.21	0.41
1:A:68:VAL:O	1:A:69:PRO:C	2.63	0.41
1:A:111:ILE:O	1:A:112:VAL:C	2.63	0.41
1:B:320:LYS:HE2	1:B:321:TYR:CZ	2.55	0.41
2:C:112:ARG:HG3	2:C:113:THR:O	2.21	0.41
3:F:83:MET:HB3	3:F:86:LEU:HD21	2.03	0.41
1:A:161:ILE:H	1:A:161:ILE:HG12	1.66	0.41
1:A:578:ASN:CG	1:A:579:PRO:C	2.89	0.41
1:B:135:ILE:HG12	1:B:149:LEU:HD22	2.01	0.41
1:B:171:GLU:HG2	1:B:172:VAL:H	1.85	0.41
1:B:270:ASP:OD1	1:B:365:THR:CB	2.55	0.41
1:B:645:ASN:C	1:B:647:LEU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:62:ILE:CG2	2:E:63:PRO:HD2	2.50	0.41
1:A:88:LEU:HD12	1:A:88:LEU:HA	1.88	0.41
1:A:566:ILE:O	1:A:567:ALA:C	2.62	0.41
1:A:567:ALA:HB1	1:A:746:ILE:CG1	2.50	0.41
1:A:862:LEU:O	1:A:863:LEU:C	2.63	0.41
1:B:269:HIS:HD2	1:B:365:THR:HG22	1.73	0.41
1:B:1209:LEU:HD21	1:B:1217:LEU:HD13	2.03	0.41
3:D:60:TYR:CE2	3:D:70:THR:HG22	2.56	0.41
3:D:150:TYR:OH	3:D:173:ALA:HB2	2.21	0.41
3:F:151:PHE:HA	3:F:152:PRO:HA	1.87	0.41
1:A:9:ASN:O	1:A:10:TYR:C	2.62	0.41
1:A:481:ILE:N	1:A:481:ILE:HD13	2.36	0.41
1:A:587:SER:O	1:A:588:SER:C	2.63	0.41
1:A:748:ASN:O	1:A:752:ASN:ND2	2.51	0.41
1:A:951:LYS:HE3	1:A:1291:TRP:CZ3	2.56	0.41
1:A:1210:GLU:HB2	1:A:1213:ASP:HB2	2.03	0.41
1:B:123:ILE:O	1:B:124:ASP:C	2.64	0.41
1:B:365:THR:O	1:B:366:TYR:C	2.63	0.41
2:C:151:GLN:HB3	2:C:158:LEU:HD21	2.03	0.41
1:A:509:ASP:HB3	1:A:510:ASN:H	1.57	0.41
1:A:809:GLU:HG3	1:A:934:TYR:CE1	2.56	0.41
1:A:810:ASP:O	1:A:813:ALA:HB3	2.21	0.41
1:A:1233:ASN:HD21	1:A:1235:CYS:HB2	1.86	0.41
1:A:1235:CYS:HA	1:A:1280:CYS:O	2.21	0.41
1:A:1269:ARG:HA	1:A:1269:ARG:HD3	1.54	0.41
1:B:163:PHE:CD1	1:B:188:PHE:HA	2.56	0.41
1:B:235:ILE:HA	1:B:286:TYR:CE2	2.55	0.41
1:B:334:ASP:O	1:B:335:LYS:C	2.63	0.41
1:B:515:ILE:O	1:B:515:ILE:HG13	2.18	0.41
1:B:749:TYR:O	1:B:753:GLN:HG2	2.21	0.41
1:B:835:ASP:O	1:B:838:LYS:N	2.54	0.41
1:B:915:GLN:HB2	1:B:1068:TRP:CH2	2.56	0.41
1:B:964:ILE:HA	1:B:1056:LYS:O	2.21	0.41
1:B:1264:SER:O	1:B:1266:TRP:N	2.54	0.41
2:C:187:LYS:O	2:C:191:GLU:HG2	2.20	0.41
3:D:82:GLN:NE2	3:D:83:MET:H	2.18	0.41
3:F:20:LEU:HD11	3:F:83:MET:CE	2.48	0.41
3:F:22:CYS:HB3	3:F:79:LEU:HB3	2.01	0.41
1:A:656:LEU:O	1:A:656:LEU:HG	2.19	0.41
1:B:484:ASP:O	1:B:485:THR:O	2.37	0.41
1:B:1135:TYR:CE1	1:B:1137:LYS:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:150:TYR:CE1	3:F:155:VAL:HG13	2.56	0.41
1:A:667:PHE:CE1	1:A:724:GLN:NE2	2.90	0.40
1:B:475:LEU:HB3	1:B:676:LEU:HD23	2.02	0.40
1:B:497:ASP:N	1:B:497:ASP:OD1	2.54	0.40
1:B:1233:ASN:HD21	1:B:1235:CYS:CB	2.35	0.40
1:B:1254:GLN:C	1:B:1255:PHE:CD2	2.99	0.40
2:C:71:SER:HA	2:C:75:PHE:HE2	1.85	0.40
3:D:144:GLY:HA2	3:D:159:TRP:CH2	2.55	0.40
1:A:405:ASN:HB3	1:A:408:ILE:HB	2.03	0.40
1:B:866:PHE:O	1:B:867:THR:C	2.63	0.40
1:A:290:PHE:CE2	1:A:321:TYR:HD2	2.39	0.40
1:B:567:ALA:HB1	1:B:746:ILE:HG13	2.02	0.40
1:B:575:ALA:C	1:B:577:LEU:N	2.79	0.40
1:B:603:PHE:C	1:B:605:GLY:HA3	2.44	0.40
1:B:870:ILE:C	1:B:872:ASN:H	2.29	0.40
1:B:1097:LEU:HD21	1:B:1223:MET:HB3	2.02	0.40
2:C:65:ARG:HA	2:C:80:SER:OG	2.21	0.40
1:A:269:HIS:CD2	1:A:269:HIS:C	2.98	0.40
1:A:306:THR:OG1	1:A:307:THR:N	2.54	0.40
1:B:36:PHE:CD1	1:B:36:PHE:N	2.89	0.40
1:B:171:GLU:HG2	1:B:172:VAL:N	2.37	0.40
1:B:275:ASP:OD1	1:B:278:GLN:NE2	2.53	0.40
1:B:651:ASP:O	1:B:651:ASP:CG	2.64	0.40
1:B:801:ILE:N	1:B:802:PRO:CD	2.84	0.40
1:B:1092:SER:O	1:B:1093:ASN:HB2	2.21	0.40
1:B:1233:ASN:OD1	1:B:1271:ILE:HG23	2.22	0.40
1:A:121:SER:H	1:A:128:LYS:HB3	1.87	0.40
1:A:474:ASP:O	1:A:475:LEU:C	2.65	0.40
1:A:573:ASN:CA	1:A:574:GLU:C	2.90	0.40
1:A:917:PHE:C	1:A:919:LEU:H	2.30	0.40
1:B:45:ILE:HA	1:B:46:PRO:HD3	1.88	0.40
1:B:520:LEU:N	1:B:520:LEU:HD13	2.36	0.40
1:B:559:PHE:CD1	1:B:560:GLU:CA	3.04	0.40
1:B:706:TRP:CG	1:B:808:LEU:HD22	2.57	0.40
1:B:985:TRP:CE2	1:B:1019:ILE:HG21	2.56	0.40
1:B:1074:LEU:HD12	1:B:1074:LEU:HA	1.93	0.40
3:D:159:TRP:CE3	3:D:200:ILE:O	2.74	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	1259/1295 (97%)	1084 (86%)	130 (10%)	45 (4%)	2	22
1	B	1259/1295 (97%)	1081 (86%)	139 (11%)	39 (3%)	3	25
2	C	214/218 (98%)	182 (85%)	30 (14%)	2 (1%)	14	45
2	E	214/218 (98%)	193 (90%)	14 (6%)	7 (3%)	3	24
3	D	215/224 (96%)	182 (85%)	24 (11%)	9 (4%)	2	19
3	F	215/224 (96%)	192 (89%)	17 (8%)	6 (3%)	4	26
All	All	3376/3474 (97%)	2914 (86%)	354 (10%)	108 (3%)	3	24

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	400	ASN
1	A	560	GLU
1	A	564	SER
1	A	566	ILE
1	A	576	LEU
1	A	606	TRP
1	A	755	THR
1	A	760	ASN
1	A	831	ILE
1	A	991	GLN
1	A	993	ILE
1	A	1169	ASN
1	A	1229	GLN
1	A	1257	ASN
1	B	209	GLY
1	B	256	LEU
1	B	560	GLU
1	B	566	ILE
1	B	576	LEU

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Mol	Chain	Res	Type
1	B	578	ASN
1	B	645	ASN
1	B	760	ASN
1	B	833	GLN
1	B	848	ASP
1	B	991	GLN
1	B	992	GLU
1	B	1167	SER
1	B	1170	LYS
1	B	1229	GLN
1	B	1274	SER
3	D	137	SER
3	D	192	SER
3	F	137	SER
3	F	138	GLY
1	A	209	GLY
1	A	210	ALA
1	A	256	LEU
1	A	399	ALA
1	A	401	PHE
1	A	540	GLY
1	A	578	ASN
1	A	645	ASN
1	A	848	ASP
1	A	1254	GLN
1	A	1258	ILE
1	A	1259	ALA
1	B	121	SER
1	B	399	ALA
1	B	980	TYR
1	B	1231	ILE
1	B	1254	GLN
3	D	30	SER
3	D	140	THR
3	D	193	SER
2	E	55	ALA
2	E	156	ASN
1	A	49	ASP
1	A	254	SER
1	A	541	LYS
1	A	577	LEU
1	A	597	ALA

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Mol	Chain	Res	Type
1	A	608	GLU
1	A	980	TYR
1	B	210	ALA
1	B	366	TYR
1	B	541	LYS
1	B	835	ASP
1	B	1094	SER
2	C	71	SER
3	D	28	THR
2	E	56	SER
2	E	71	SER
3	F	140	THR
3	F	175	LEU
3	F	192	SER
1	A	563	LYS
1	A	567	ALA
1	A	589	ASP
1	A	970	ASN
1	A	1094	SER
1	A	1146	THR
1	B	124	ASP
1	B	400	ASN
1	B	561	HIS
1	B	757	GLU
1	B	761	ASN
1	B	1257	ASN
3	D	154	PRO
3	F	135	SER
1	A	475	LEU
1	A	644	GLY
1	A	1147	ASN
1	B	763	ASN
1	B	970	ASN
3	D	133	SER
2	E	16	GLY
2	E	175	SER
2	E	187	LYS
1	A	1242	ASN
1	B	572	VAL
1	B	831	ILE
1	B	1147	ASN
2	C	15	PRO

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Mol	Chain	Res	Type
1	B	494	ILE
1	A	572	VAL
1	B	685	ILE
3	D	151	PHE

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	1124/1178 (95%)	1015 (90%)	109 (10%)	8	29
1	B	1124/1178 (95%)	1028 (92%)	96 (8%)	10	33
2	C	186/190 (98%)	160 (86%)	26 (14%)	3	18
2	E	186/190 (98%)	165 (89%)	21 (11%)	5	23
3	D	181/190 (95%)	159 (88%)	22 (12%)	5	21
3	F	181/190 (95%)	165 (91%)	16 (9%)	9	33
All	All	2982/3116 (96%)	2692 (90%)	290 (10%)	8	29

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	24	ILE
1	A	30	MET
1	A	31	GLN
1	A	45	ILE
1	A	66	LYS
1	A	106	MET
1	A	122	THR
1	A	123	ILE
1	A	147	GLU
1	A	154	ILE
1	A	157	SER
1	A	161	ILE
1	A	165	CYS

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Mol	Chain	Res	Type
1	A	200	LEU
1	A	202	VAL
1	A	204	THR
1	A	208	LEU
1	A	254	SER
1	A	258	VAL
1	A	269	HIS
1	A	276	SER
1	A	297	LEU
1	A	336	LEU
1	A	363	ARG
1	A	365	THR
1	A	373	VAL
1	A	386	ILE
1	A	411	MET
1	A	412	ASN
1	A	422	LEU
1	A	480	GLU
1	A	493	ASN
1	A	494	ILE
1	A	506	PHE
1	A	507	ASN
1	A	509	ASP
1	A	536	ARG
1	A	549	THR
1	A	569	THR
1	A	570	ASN
1	A	580	SER
1	A	591	VAL
1	A	598	THR
1	A	602	MET
1	A	607	VAL
1	A	622	SER
1	A	627	ILE
1	A	643	ILE
1	A	651	ASP
1	A	656	LEU
1	A	671	ILE
1	A	681	LEU
1	A	689	VAL
1	A	707	ASP
1	A	734	GLU

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Mol	Chain	Res	Type
1	A	748	ASN
1	A	750	GLN
1	A	753	GLN
1	A	762	ILE
1	A	763	ASN
1	A	766	ILE
1	A	768	ASP
1	A	771	SER
1	A	776	SER
1	A	792	SER
1	A	794	SER
1	A	799	SER
1	A	807	ARG
1	A	829	THR
1	A	845	LEU
1	A	846	SER
1	A	847	THR
1	A	860	GLN
1	A	873	ILE
1	A	896	SER
1	A	922	SER
1	A	923	LYS
1	A	928	LEU
1	A	956	ILE
1	A	958	LEU
1	A	970	ASN
1	A	994	LYS
1	A	1015	ILE
1	A	1021	ASN
1	A	1023	ARG
1	A	1024	LEU
1	A	1026	ASN
1	A	1042	SER
1	A	1069	ILE
1	A	1082	LYS
1	A	1092	SER
1	A	1130	ILE
1	A	1131	ARG
1	A	1140	ARG
1	A	1143	VAL
1	A	1146	THR
1	A	1150	LEU

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Mol	Chain	Res	Type
1	A	1152	SER
1	A	1172	ASN
1	A	1211	ILE
1	A	1213	ASP
1	A	1218	SER
1	A	1219	GLN
1	A	1228	ASP
1	A	1229	GLN
1	A	1255	PHE
1	A	1269	ARG
1	A	1283	GLU
1	B	5	ASN
1	B	14	VAL
1	B	24	ILE
1	B	27	VAL
1	B	51	PHE
1	B	66	LYS
1	B	106	MET
1	B	123	ILE
1	B	126	GLU
1	B	143	SER
1	B	147	GLU
1	B	154	ILE
1	B	157	SER
1	B	161	ILE
1	B	165	CYS
1	B	200	LEU
1	B	202	VAL
1	B	204	THR
1	B	253	MET
1	B	254	SER
1	B	258	VAL
1	B	269	HIS
1	B	272	LYS
1	B	297	LEU
1	B	306	THR
1	B	310	LEU
1	B	340	LYS
1	B	363	ARG
1	B	373	VAL
1	B	411	MET
1	B	497	ASP

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Mol	Chain	Res	Type
1	B	507	ASN
1	B	517	ILE
1	B	520	LEU
1	B	568	LEU
1	B	573	ASN
1	B	580	SER
1	B	584	THR
1	B	591	VAL
1	B	598	THR
1	B	599	GLU
1	B	602	MET
1	B	613	ASP
1	B	627	ILE
1	B	662	VAL
1	B	663	ILE
1	B	671	ILE
1	B	675	VAL
1	B	689	VAL
1	B	748	ASN
1	B	750	GLN
1	B	752	ASN
1	B	773	LEU
1	B	776	SER
1	B	807	ARG
1	B	811	PHE
1	B	814	SER
1	B	827	ARG
1	B	829	THR
1	B	838	LYS
1	B	846	SER
1	B	873	ILE
1	B	874	ILE
1	B	889	ILE
1	B	900	ILE
1	B	919	LEU
1	B	922	SER
1	B	923	LYS
1	B	928	LEU
1	B	943	THR
1	B	956	ILE
1	B	986	THR
1	B	1006	ASN

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Mol	Chain	Res	Type
1	B	1021	ASN
1	B	1023	ARG
1	B	1026	ASN
1	B	1090	ASN
1	B	1092	SER
1	B	1128	VAL
1	B	1130	ILE
1	B	1131	ARG
1	B	1143	VAL
1	B	1148	ILE
1	B	1172	ASN
1	B	1199	GLN
1	B	1211	ILE
1	B	1228	ASP
1	B	1232	THR
1	B	1233	ASN
1	B	1253	HIS
1	B	1255	PHE
1	B	1265	ASN
1	B	1275	SER
1	B	1283	GLU
1	B	1287	VAL
1	B	1294	ARG
2	C	13	LEU
2	C	14	SER
2	C	24	ARG
2	C	52	ILE
2	C	58	LEU
2	C	67	SER
2	C	76	THR
2	C	85	GLU
2	C	87	PHE
2	C	89	VAL
2	C	101	THR
2	C	111	LYS
2	C	126	ASP
2	C	129	LEU
2	C	139	LEU
2	C	146	ARG
2	C	158	LEU
2	C	169	GLU
2	C	172	SER

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Mol	Chain	Res	Type
2	C	174	ASP
2	C	178	SER
2	C	179	LEU
2	C	186	SER
2	C	210	THR
2	C	212	SER
2	C	214	ASN
3	D	3	GLN
3	D	4	LEU
3	D	6	GLU
3	D	21	SER
3	D	43	LYS
3	D	62	ASP
3	D	64	VAL
3	D	67	ARG
3	D	69	THR
3	D	89	GLU
3	D	91	THR
3	D	110	GLN
3	D	115	THR
3	D	122	LYS
3	D	132	SER
3	D	174	VAL
3	D	182	SER
3	D	184	SER
3	D	192	SER
3	D	206	LYS
3	D	211	LYS
3	D	212	VAL
2	E	1	GLU
2	E	12	SER
2	E	14	SER
2	E	29	VAL
2	E	54	ARG
2	E	56	SER
2	E	76	THR
2	E	87	PHE
2	E	101	THR
2	E	107	LYS
2	E	113	THR
2	E	118	SER
2	E	139	LEU

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Mol	Chain	Res	Type
2	E	158	LEU
2	E	166	SER
2	E	169	GLU
2	E	174	ASP
2	E	182	THR
2	E	185	LEU
2	E	195	VAL
2	E	214	ASN
3	F	5	GLN
3	F	6	GLU
3	F	43	LYS
3	F	62	ASP
3	F	63	SER
3	F	65	GLU
3	F	67	ARG
3	F	110	GLN
3	F	118	SER
3	F	122	LYS
3	F	135	SER
3	F	174	VAL
3	F	184	SER
3	F	204	ASN
3	F	211	LYS
3	F	217	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	26	ASN
1	A	39	HIS
1	A	53	ASN
1	A	67	GLN
1	A	162	GLN
1	A	170	HIS
1	A	205	ASN
1	A	238	ASN
1	A	311	GLN
1	A	315	ASN
1	A	353	ASN
1	A	383	ASN
1	A	412	ASN

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Mol	Chain	Res	Type
1	A	493	ASN
1	A	609	GLN
1	A	642	ASN
1	A	687	ASN
1	A	722	ASN
1	A	748	ASN
1	A	774	ASN
1	A	905	ASN
1	A	940	ASN
1	A	960	ASN
1	A	966	ASN
1	A	1006	ASN
1	A	1021	ASN
1	A	1176	ASN
1	A	1196	ASN
1	A	1233	ASN
1	A	1253	HIS
1	A	1256	ASN
1	A	1265	ASN
1	B	26	ASN
1	B	29	GLN
1	B	39	HIS
1	B	40	ASN
1	B	67	GLN
1	B	139	GLN
1	B	238	ASN
1	B	246	ASN
1	B	269	HIS
1	B	311	GLN
1	B	383	ASN
1	B	642	ASN
1	B	833	GLN
1	B	843	ASN
1	B	860	GLN
1	B	988	GLN
1	B	1051	ASN
1	B	1064	HIS
1	B	1090	ASN
1	B	1106	GLN
1	B	1172	ASN
1	B	1196	ASN
1	B	1227	ASN

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Mol	Chain	Res	Type
1	B	1229	GLN
1	B	1233	ASN
1	B	1254	GLN
1	B	1256	ASN
2	C	57	ASN
2	C	142	ASN
2	C	156	ASN
2	C	164	GLN
2	C	202	HIS
2	C	214	ASN
3	D	5	GLN
3	D	39	GLN
3	D	82	GLN
3	D	84	ASN
2	E	34	HIS
2	E	41	GLN
2	E	128	GLN
2	E	156	ASN
2	E	202	HIS
3	F	110	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1267/1295 (97%)	-0.22	7 (0%) 85 68	29, 84, 98, 110	0
1	B	1267/1295 (97%)	-0.22	3 (0%) 91 81	33, 85, 97, 111	0
2	C	216/218 (99%)	-0.05	3 (1%) 73 51	62, 84, 92, 95	0
2	E	216/218 (99%)	-0.17	2 (0%) 81 60	67, 85, 92, 95	0
3	D	217/224 (96%)	-0.26	0 100 100	75, 85, 95, 103	0
3	F	217/224 (96%)	-0.24	2 (0%) 81 60	72, 84, 92, 99	0
All	All	3400/3474 (97%)	-0.21	17 (0%) 87 71	29, 84, 97, 111	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	TYR	3.9
2	C	171	ASP	3.0
1	A	493	ASN	2.7
1	A	989	ASP	2.6
1	A	529	GLU	2.5
1	A	1063	THR	2.5
2	E	216	GLY	2.5
3	F	2	VAL	2.4
1	A	512	PRO	2.3
1	B	671	ILE	2.2
2	C	138	CYS	2.2
1	B	762	ILE	2.2
1	B	1063	THR	2.2
3	F	217	GLU	2.1
1	A	507	ASN	2.1
2	C	176	THR	2.1
2	E	171	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	A	1297	1/1	0.79	0.09	101,101,101,101	0
5	CA	B	1298	1/1	0.93	0.07	110,110,110,110	0
4	ZN	A	1	1/1	0.97	0.07	81,81,81,81	0
4	ZN	B	1297	1/1	0.99	0.11	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.