



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:30 AM UTC

PDB ID : 1ZM3 / pdb_00001zm3
Title : Structure of the apo eEF2-ETA complex
Authors : Joergensen, R.; Merrill, A.R.; Yates, S.P.; Marquez, V.E.; Schwan, A.L.; Boesen, T.; Andersen, G.R.
Deposited on : 2005-05-10
Resolution : 3.07 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

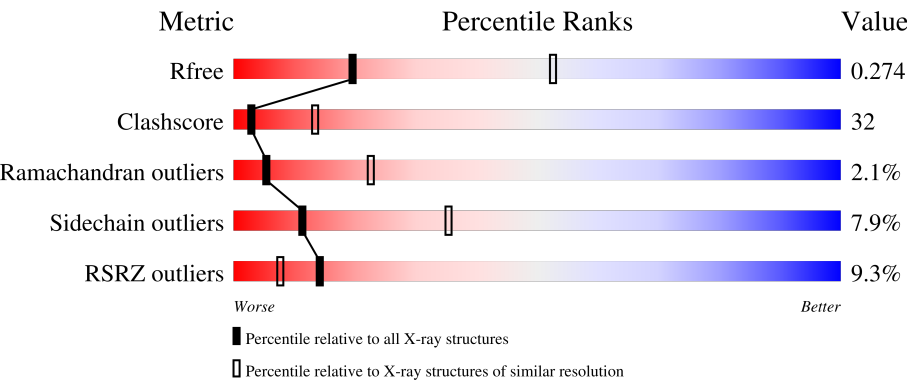
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.07 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	842	% 50%44% . .
1	C	842	7% 41%48%8% . .
1	E	842	24% 42%50%6% .
2	B	207	3% 54%37%9% .
2	D	207	2% 49%43%6% .

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Mol	Chain	Length	Quality of chain
2	F	207	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '2%', followed by a green segment labeled '53%', a yellow segment labeled '37%', and a small orange segment at the end labeled '10%'.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23979 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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	C	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	E	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	699	DDE	HIS	modified residue	UNP P32324
C	699	DDE	HIS	modified residue	UNP P32324
E	699	DDE	HIS	modified residue	UNP P32324

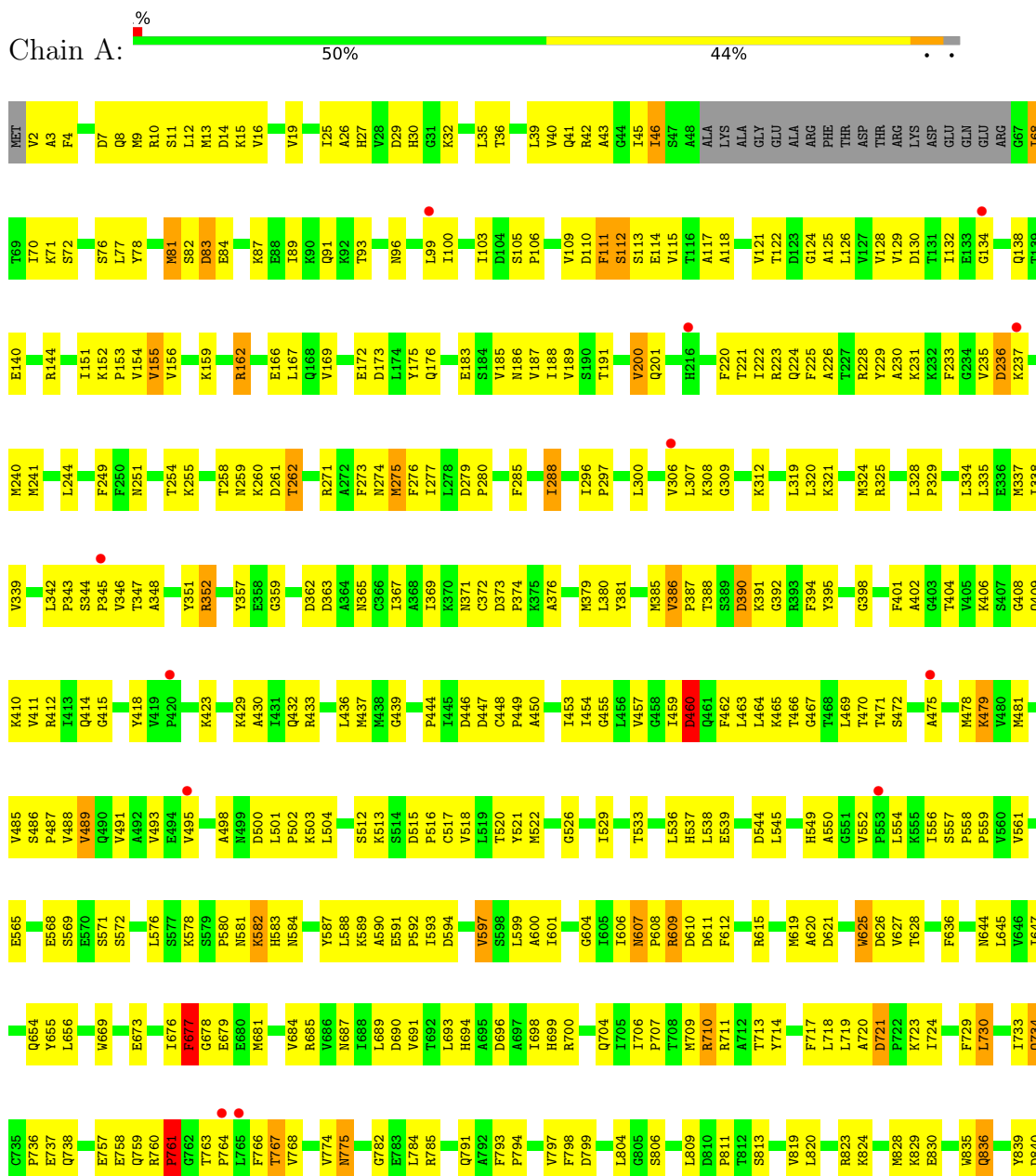
- Molecule 2 is a protein called exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	D	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	F	207	Total	C	N	O	0	0	0
			1588	1001	283	304			

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.

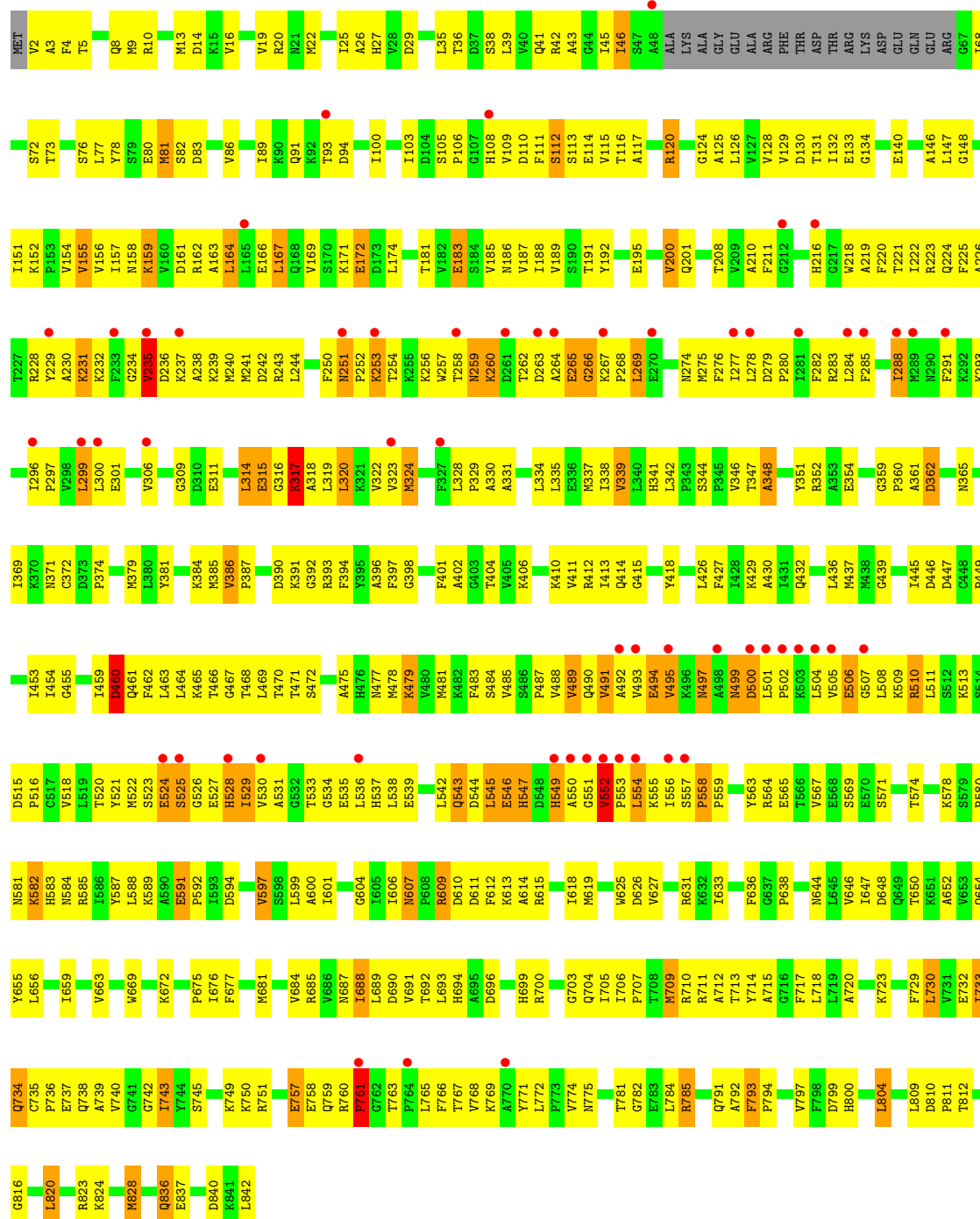
• Molecule 1: Elongation factor 2



K841
L842

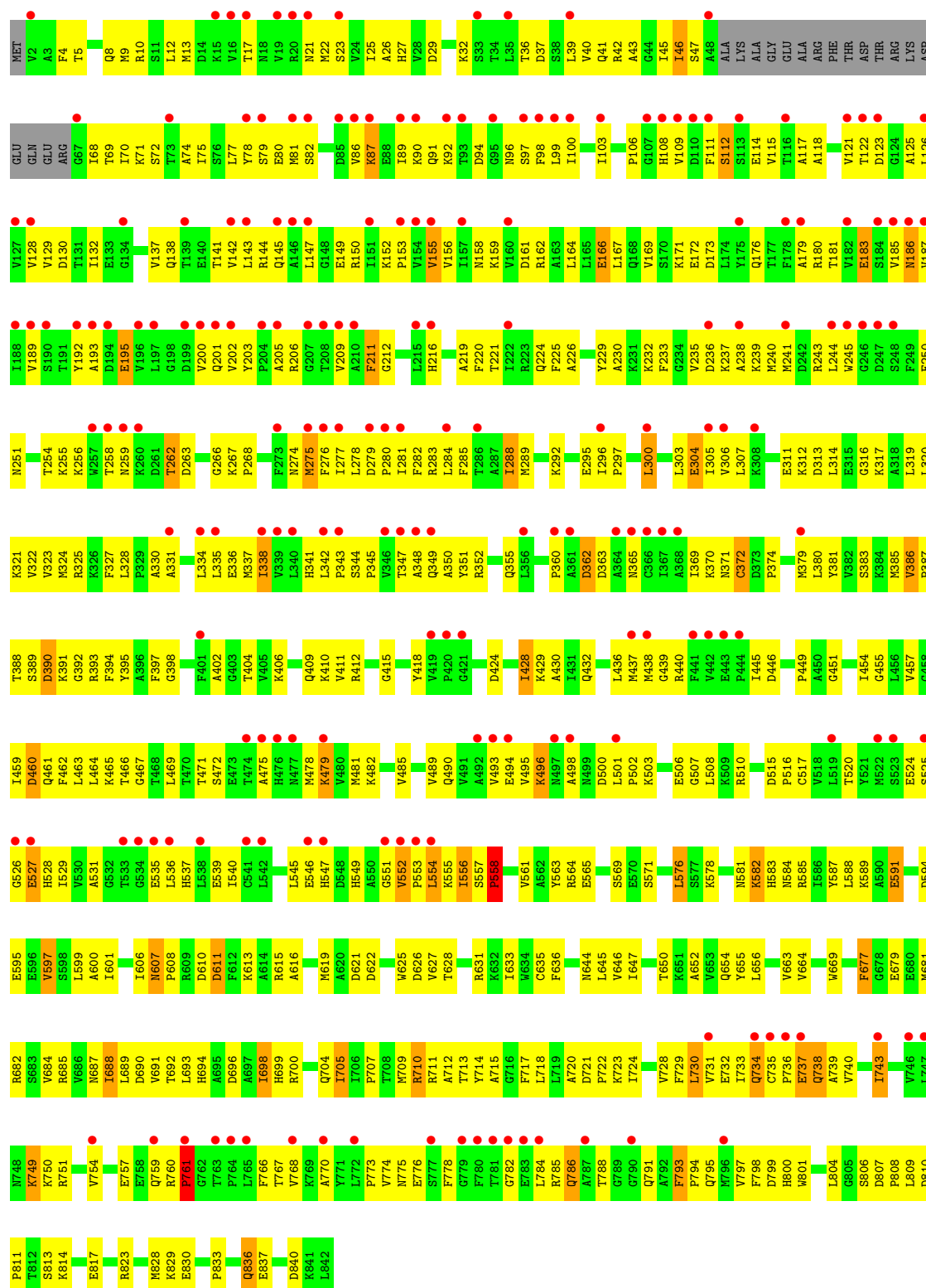
• Molecule 1: Elongation factor 2

Chain C: 7% 41% 48% 8% ..



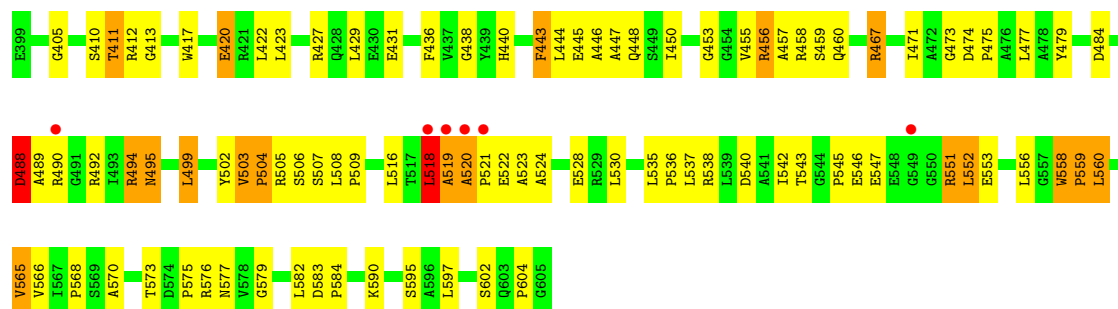
• Molecule 1: Elongation factor 2

Chain E: 24% 42% 50% 6% .



● Molecule 2: exotoxin A





• Molecule 2: exotoxin A



• Molecule 2: exotoxin A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	329.43Å 69.09Å 190.80Å 90.00° 103.46° 90.00°	Depositor
Resolution (Å)	40.00 – 3.07 40.00 – 3.07	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.07) 97.7 (40.00-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.282 0.243 , 0.274	Depositor DCC
R_{free} test set	1571 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23979	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7793e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: DDE

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	0.57	0/6517	1.03	19/8823 (0.2%)
1	C	0.61	4/6517 (0.1%)	1.09	43/8823 (0.5%)
1	E	0.54	0/6517	1.01	29/8823 (0.3%)
2	B	0.79	0/1627	1.23	16/2216 (0.7%)
2	D	0.83	0/1627	1.21	14/2216 (0.6%)
2	F	0.73	1/1627 (0.1%)	1.23	12/2216 (0.5%)
All	All	0.62	5/24432 (0.0%)	1.08	133/33117 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	543	GLN	CG-CD	5.60	1.66	1.52
2	F	578	VAL	CA-CB	-5.38	1.49	1.54
1	C	688	ILE	CA-CB	5.33	1.59	1.53
1	C	709	MET	SD-CE	-5.20	1.66	1.79
1	C	543	GLN	CD-OE1	-5.05	1.14	1.23

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	554	LEU	N-CA-C	10.67	125.04	109.14
1	C	591	GLU	CA-C-N	9.03	128.97	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	591	GLU	C-N-CA	9.03	128.97	119.85
1	E	591	GLU	CA-C-N	8.81	128.75	119.85
1	E	591	GLU	C-N-CA	8.81	128.75	119.85
1	C	582	LYS	N-CA-C	-8.21	101.33	113.40
1	E	498	ALA	N-CA-C	8.20	121.81	111.24
1	A	236	ASP	N-CA-C	-8.14	96.01	108.96
1	C	251	ASN	CA-C-N	8.07	127.79	119.64
1	C	251	ASN	C-N-CA	8.07	127.79	119.64
2	F	587	ILE	N-CA-C	-7.92	99.76	107.76
1	A	115	VAL	N-CA-C	-7.81	103.19	110.53
1	A	721	ASP	CA-C-N	7.81	127.57	119.76
1	A	721	ASP	C-N-CA	7.81	127.57	119.76
2	B	570	ALA	N-CA-C	-7.68	103.97	112.72
1	C	505	VAL	N-CA-C	-7.25	103.14	113.07
1	C	545	LEU	N-CA-C	-7.23	103.34	111.07
1	C	115	VAL	N-CA-C	-7.09	103.86	110.53
2	B	411	THR	N-CA-C	-7.06	103.63	111.82
1	E	471	THR	N-CA-C	-7.05	106.58	114.62
1	A	415	GLY	CA-C-N	7.04	126.56	119.24
1	A	415	GLY	C-N-CA	7.04	126.56	119.24
2	F	438	GLY	N-CA-C	6.97	119.96	110.69
2	B	488	ASP	N-CA-C	-6.94	101.58	110.53
2	B	504	PRO	N-CA-C	-6.88	100.41	110.80
1	C	552	VAL	CA-C-N	6.85	127.79	120.11
1	C	552	VAL	C-N-CA	6.85	127.79	120.11
1	E	195	GLU	CG-CD-OE2	-6.79	102.77	118.40
1	A	593	ILE	N-CA-C	-6.68	98.57	108.85
1	C	348	ALA	N-CA-C	6.60	118.56	111.36
1	C	471	THR	N-CA-C	-6.56	107.14	114.62
2	F	595	SER	N-CA-C	6.53	120.16	112.72
2	F	517	THR	N-CA-C	-6.51	102.14	110.53
1	C	22	MET	N-CA-C	6.48	118.00	108.86
2	D	518	LEU	N-CA-C	6.48	124.61	110.80
2	F	518	LEU	N-CA-C	6.46	123.09	110.56
2	F	587	ILE	CB-CA-C	-6.44	103.82	110.71
2	D	570	ALA	N-CA-C	-6.35	105.28	113.16
1	C	546	GLU	N-CA-C	6.35	119.14	111.40
1	E	386	VAL	CA-C-N	6.34	126.29	119.76
1	E	386	VAL	C-N-CA	6.34	126.29	119.76
2	F	573	THR	N-CA-C	-6.32	100.62	110.42
1	E	793	PHE	CA-C-N	6.29	126.20	119.85
1	E	793	PHE	C-N-CA	6.29	126.20	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	705	ILE	N-CA-C	6.28	116.44	110.53
1	C	543	GLN	OE1-CD-NE2	6.27	128.87	122.60
2	F	486	GLU	CA-C-N	6.27	126.63	119.92
2	F	486	GLU	C-N-CA	6.27	126.63	119.92
2	D	520	ALA	N-CA-C	6.26	118.59	110.40
1	C	386	VAL	CA-C-N	6.21	126.54	119.83
1	C	386	VAL	C-N-CA	6.21	126.54	119.83
1	C	315	GLU	N-CA-C	6.21	118.50	108.32
1	E	115	VAL	N-CA-C	-6.19	104.72	110.53
1	C	155	VAL	N-CA-C	6.18	118.04	109.45
1	C	733	ILE	N-CA-C	6.11	116.67	108.11
2	F	411	THR	N-CA-C	-6.09	104.71	111.71
2	B	579	GLY	N-CA-C	-5.97	107.37	114.48
1	A	386	VAL	CA-C-N	5.92	126.11	119.90
1	A	386	VAL	C-N-CA	5.92	126.11	119.90
1	E	721	ASP	CA-C-N	5.88	125.79	119.85
1	E	721	ASP	C-N-CA	5.88	125.79	119.85
1	A	793	PHE	CA-C-N	5.86	126.35	120.14
1	A	793	PHE	C-N-CA	5.86	126.35	120.14
1	A	839	TYR	N-CA-C	-5.86	103.21	110.41
2	B	519	ALA	N-CA-C	5.85	123.26	110.80
2	D	573	THR	N-CA-C	-5.84	101.88	110.52
1	E	582	LYS	N-CA-C	-5.83	104.83	113.40
1	C	510	ARG	N-CA-C	-5.83	105.83	113.12
1	E	652	ALA	N-CA-C	5.83	119.43	111.39
1	C	386	VAL	N-CA-C	5.79	114.20	107.89
1	A	275	MET	N-CA-C	5.79	118.46	111.40
1	A	288	ILE	N-CA-C	5.78	116.43	110.36
1	C	317	LYS	N-CA-C	-5.75	105.36	112.38
2	B	520	ALA	CA-C-N	5.73	125.10	118.85
2	B	520	ALA	C-N-CA	5.73	125.10	118.85
1	E	155	VAL	N-CA-C	5.72	117.57	108.87
2	D	537	LEU	N-CA-C	-5.71	102.99	110.53
1	E	705	ILE	N-CA-C	5.68	116.45	110.72
1	C	636	PHE	N-CA-C	-5.66	101.81	110.14
1	E	830	GLU	N-CA-C	5.65	118.99	111.75
2	F	570	ALA	N-CA-C	-5.64	106.25	113.02
1	C	607	ASN	CA-C-N	5.63	125.47	119.28
1	C	607	ASN	C-N-CA	5.63	125.47	119.28
2	D	519	ALA	N-CA-C	5.61	122.75	110.80
1	A	706	ILE	CB-CA-C	-5.61	108.37	113.70
1	E	415	GLY	CA-C-N	5.61	125.07	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	415	GLY	C-N-CA	5.61	125.07	119.24
1	A	471	THR	N-CA-C	-5.59	108.25	114.62
2	D	413	GLY	CA-C-O	-5.59	117.81	122.33
1	C	793	PHE	CA-C-N	5.58	125.53	119.78
1	C	793	PHE	C-N-CA	5.58	125.53	119.78
2	F	457	ALA	N-CA-C	-5.58	103.01	110.55
2	B	443	PHE	N-CA-C	5.56	118.71	110.48
1	E	611	ASP	N-CA-C	-5.55	100.94	109.76
1	E	288	ILE	N-CA-C	5.54	116.27	110.62
2	B	503	VAL	N-CA-CB	5.52	115.64	111.83
2	B	595	SER	N-CA-C	5.50	119.56	112.41
1	E	554	LEU	N-CA-C	5.46	117.48	109.24
1	C	259	ASN	N-CA-C	-5.41	107.33	114.31
2	D	504	PRO	N-CA-C	-5.38	101.79	110.55
1	C	652	ALA	N-CA-C	5.36	118.97	111.74
1	A	607	ASN	CA-C-N	5.35	125.17	119.28
1	A	607	ASN	C-N-CA	5.35	125.17	119.28
1	C	547	HIS	N-CA-C	5.33	118.25	111.69
2	B	558	TRP	CA-C-N	-5.29	113.23	119.84
2	B	558	TRP	C-N-CA	-5.29	113.23	119.84
1	E	714	TYR	N-CA-C	-5.29	105.60	111.36
1	C	267	LYS	CA-C-N	5.28	125.21	119.78
1	C	267	LYS	C-N-CA	5.28	125.21	119.78
1	C	415	GLY	CA-C-N	5.27	125.33	119.32
1	C	415	GLY	C-N-CA	5.27	125.33	119.32
1	E	733	ILE	N-CA-C	5.21	115.62	108.12
1	C	260	LYS	N-CA-C	-5.20	102.79	110.48
1	E	607	ASN	CA-C-N	5.20	125.24	119.32
1	E	607	ASN	C-N-CA	5.20	125.24	119.32
2	D	437	VAL	CB-CA-C	-5.19	105.02	110.62
2	B	573	THR	N-CA-C	-5.19	102.84	110.52
1	A	155	VAL	N-CA-C	5.18	117.16	109.17
2	D	432	ARG	N-CA-C	-5.18	106.65	113.17
1	C	288	ILE	N-CA-C	5.12	115.74	110.36
1	E	607	ASN	N-CA-C	5.11	117.61	109.64
2	D	603	GLN	CA-C-N	5.09	126.21	119.84
2	D	603	GLN	C-N-CA	5.09	126.21	119.84
1	E	496	LYS	N-CA-C	-5.08	106.49	113.30
2	B	518	LEU	N-CA-C	5.08	121.62	110.80
2	B	565	VAL	N-CA-C	-5.08	100.21	107.78
1	C	359	GLY	CA-C-N	5.08	125.31	119.83
1	C	359	GLY	C-N-CA	5.08	125.31	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	VAL	N-CA-C	5.07	115.61	108.36
1	E	622	ASP	N-CA-C	5.05	119.07	113.01
1	C	574	THR	N-CA-C	5.04	117.35	110.24
1	C	339	VAL	N-CA-C	5.03	115.26	110.53
2	D	406	ASP	N-CA-C	5.01	117.74	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	195	GLU	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6405	0	6472	369	0
1	C	6405	0	6472	487	0
1	E	6405	0	6472	462	0
2	B	1588	0	1539	93	0
2	D	1588	0	1539	80	0
2	F	1588	0	1539	75	0
All	All	23979	0	24033	1552	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 32.

All (1552) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LYS:HG2	1:C:392:GLY:H	1.13	1.11
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.32	1.11
1:E:556:ILE:HG22	1:E:557:SER:H	1.10	1.10
1:A:16:VAL:HG13	1:A:345:PRO:HG2	1.33	1.09
1:C:253:LYS:HE3	1:C:253:LYS:HA	1.35	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:VAL:HG22	1:E:553:PRO:HD3	1.36	1.05
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.37	1.03
1:C:231:LYS:HE3	1:C:232:LYS:HG3	1.40	1.02
1:E:10:ARG:HH12	1:E:449:PRO:CD	1.75	0.99
1:C:820:LEU:O	1:C:824:LYS:HG3	1.63	0.98
2:F:546:GLU:HG3	2:F:547:GLU:HG3	1.43	0.97
1:A:16:VAL:CG1	1:A:345:PRO:HG2	1.92	0.97
1:C:404:THR:HG22	1:C:449:PRO:HA	1.43	0.96
1:E:552:VAL:HG22	1:E:553:PRO:CD	1.94	0.96
1:A:737:GLU:HG3	1:A:766:PHE:CE2	2.01	0.94
1:E:694:HIS:HD2	1:E:696:ASP:H	1.06	0.94
1:C:265:GLU:HG3	1:C:266:GLY:H	1.29	0.94
1:E:535:GLU:OE2	1:E:778:PHE:HA	1.68	0.94
1:C:42:ARG:HG3	1:C:331:ALA:CB	1.98	0.93
1:A:627:VAL:HG12	2:F:405:GLY:HA2	1.51	0.93
1:C:552:VAL:HG22	1:C:553:PRO:CD	1.99	0.93
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.50	0.92
1:A:533:THR:H	1:A:537:HIS:CD2	1.88	0.92
1:A:533:THR:H	1:A:537:HIS:HD2	1.16	0.91
1:C:578:LYS:HE2	1:C:840:ASP:OD1	1.70	0.91
2:D:546:GLU:HG3	2:D:547:GLU:HG3	1.52	0.91
1:C:256:LYS:HD3	1:C:257:TRP:H	1.36	0.90
1:C:256:LYS:HE2	1:C:256:LYS:HA	1.51	0.90
1:E:91:GLN:HE22	1:E:344:SER:H	1.16	0.90
1:C:681:MET:HE2	1:C:717:PHE:CD1	2.05	0.90
2:D:520:ALA:HB3	2:D:522:GLU:OE2	1.71	0.90
1:C:836:GLN:H	1:C:836:GLN:HE21	1.20	0.88
1:A:578:LYS:HE3	1:A:840:ASP:OD1	1.73	0.88
1:C:694:HIS:HD2	1:C:696:ASP:H	1.18	0.88
1:E:27:HIS:HD2	1:E:29:ASP:H	1.16	0.88
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.04	0.87
1:A:229:TYR:CE2	1:A:276:PHE:HB3	2.08	0.87
1:C:506:GLU:HG3	1:C:510:ARG:NE	1.88	0.87
1:C:315:GLU:HA	1:C:319:LEU:HB2	1.56	0.87
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.54	0.87
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.55	0.87
1:A:404:THR:HG22	1:A:449:PRO:HA	1.55	0.86
1:C:225:PHE:CD2	1:C:277:ILE:HG13	2.11	0.86
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.58	0.85
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.58	0.85
1:E:404:THR:HG22	1:E:449:PRO:HA	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:546:GLU:HB3	1:E:554:LEU:HD12	1.56	0.85
1:A:694:HIS:HD2	1:A:696:ASP:H	1.18	0.85
1:C:391:LYS:HG2	1:C:392:GLY:N	1.88	0.85
1:A:71:LYS:HB3	1:A:386:VAL:HG23	1.60	0.84
1:E:694:HIS:O	1:E:700:ARG:HD3	1.77	0.84
1:C:545:LEU:O	1:C:550:ALA:HB3	1.77	0.84
1:A:584:ASN:HD22	1:A:693:LEU:HA	1.40	0.84
2:B:552:LEU:HD12	2:B:552:LEU:H	1.43	0.84
2:B:520:ALA:HB3	2:B:522:GLU:OE2	1.77	0.83
1:E:10:ARG:HH12	1:E:449:PRO:HD2	1.40	0.83
1:E:556:ILE:HG22	1:E:557:SER:N	1.92	0.83
2:D:531:ILE:HD11	2:D:533:HIS:O	1.77	0.83
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.59	0.83
2:D:488:ASP:OD2	2:D:490:ARG:HG2	1.79	0.83
1:C:504:LEU:O	1:C:508:LEU:HG	1.79	0.82
1:E:503:LYS:HB3	1:E:551:GLY:HA3	1.60	0.82
1:E:482:LYS:HD3	1:E:797:VAL:HG11	1.62	0.82
1:C:296:ILE:HD13	1:C:319:LEU:HD21	1.61	0.82
1:E:71:LYS:HE3	1:E:387:PRO:CD	2.09	0.82
1:A:132:ILE:HD12	1:A:162:ARG:HH11	1.44	0.82
1:C:314:LEU:HD11	1:C:318:ALA:HB1	1.62	0.82
1:E:694:HIS:CD2	1:E:696:ASP:H	1.95	0.82
1:A:737:GLU:HG3	1:A:766:PHE:HE2	1.41	0.81
2:D:546:GLU:CG	2:D:547:GLU:HG3	2.09	0.81
1:C:552:VAL:HG22	1:C:553:PRO:HD2	1.61	0.81
1:E:237:LYS:HA	1:E:240:MET:HB3	1.61	0.81
1:E:155:VAL:HG23	1:E:202:VAL:HG11	1.62	0.81
1:C:229:TYR:CE2	1:C:276:PHE:HB3	2.16	0.81
1:E:289:MET:HE1	1:E:316:GLY:C	2.05	0.81
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.61	0.81
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.62	0.81
1:A:27:HIS:HD2	1:A:29:ASP:H	1.27	0.80
1:A:820:LEU:HD11	1:A:830:GLU:HG2	1.64	0.80
1:A:500:ASP:HB2	1:A:552:VAL:HG11	1.64	0.80
1:A:694:HIS:O	1:A:700:ARG:HD3	1.82	0.80
1:A:132:ILE:HD12	1:A:162:ARG:CD	2.12	0.80
2:D:531:ILE:HD12	2:D:533:HIS:CE1	2.17	0.80
1:C:391:LYS:CG	1:C:392:GLY:H	1.94	0.79
1:E:147:LEU:CD1	1:E:192:TYR:HB2	2.12	0.79
1:C:191:THR:O	1:C:763:THR:HG22	1.80	0.79
1:A:45:ILE:HD12	1:A:76:SER:HB3	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:417:TRP:CE2	2:D:568:PRO:HB2	2.17	0.79
1:A:140:GLU:HG3	1:A:188:ILE:CD1	2.12	0.79
1:C:591:GLU:O	1:C:685:ARG:HB3	1.81	0.79
1:E:27:HIS:CD2	1:E:29:ASP:H	2.01	0.79
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.64	0.79
1:E:459:ILE:HG21	1:E:463:LEU:HD12	1.65	0.79
2:B:417:TRP:CE2	2:B:568:PRO:HB2	2.17	0.78
2:D:527:VAL:O	2:D:531:ILE:HG23	1.84	0.78
2:B:552:LEU:HD12	2:B:552:LEU:N	1.97	0.78
1:C:836:GLN:H	1:C:836:GLN:NE2	1.81	0.78
1:E:10:ARG:HH12	1:E:449:PRO:HD3	1.48	0.78
1:A:654:GLN:HG2	1:A:655:TYR:CD2	2.18	0.78
2:D:527:VAL:HG13	2:D:542:ILE:HD12	1.65	0.78
1:C:157:ILE:CD1	1:C:181:THR:HG21	2.14	0.78
1:E:46:ILE:HG22	1:E:47:SER:H	1.49	0.78
2:D:458:ARG:H	2:D:460:GLN:HE21	1.28	0.77
2:F:488:ASP:OD2	2:F:492:ARG:HB2	1.84	0.77
1:A:647:ILE:HG13	1:A:685:ARG:HE	1.49	0.77
1:C:544:ASP:HB3	1:C:549:HIS:CD2	2.20	0.77
1:E:300:LEU:HG	1:E:305:ILE:HB	1.67	0.77
1:C:258:THR:HG22	1:C:260:LYS:H	1.47	0.77
1:E:615:ARG:HG2	1:E:619:MET:HE2	1.65	0.77
2:F:417:TRP:CE2	2:F:568:PRO:HB2	2.19	0.77
2:F:513:ARG:HB2	2:F:513:ARG:HH11	1.47	0.76
1:C:265:GLU:HG3	1:C:266:GLY:N	1.96	0.76
1:C:659:ILE:O	1:C:663:VAL:HG23	1.84	0.76
1:A:16:VAL:HG13	1:A:345:PRO:CG	2.14	0.76
1:C:2:VAL:HG22	1:C:3:ALA:H	1.51	0.76
1:E:495:VAL:HG12	1:E:554:LEU:HD23	1.67	0.76
1:C:536:LEU:HD12	1:C:537:HIS:N	2.01	0.75
1:E:238:ALA:O	1:E:241:MET:HG2	1.86	0.75
1:E:694:HIS:HD2	1:E:696:ASP:N	1.83	0.75
1:A:465:LYS:HD2	1:A:517:CYS:SG	2.27	0.75
1:E:581:ASN:HD21	1:E:704:GLN:HG3	1.52	0.75
2:B:455:VAL:C	2:B:456:ARG:HD2	2.12	0.75
1:C:584:ASN:HD22	1:C:693:LEU:HA	1.52	0.75
1:C:552:VAL:HG22	1:C:553:PRO:HD3	1.65	0.74
1:E:334:LEU:O	1:E:338:ILE:HG12	1.86	0.74
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.22	0.74
1:E:152:LYS:HD2	1:E:200:VAL:CG2	2.17	0.74
1:E:152:LYS:HD2	1:E:200:VAL:HG23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ILE:HG13	1:A:455:GLY:H	1.53	0.74
1:A:533:THR:N	1:A:537:HIS:HD2	1.85	0.74
1:C:27:HIS:HD2	1:C:29:ASP:H	1.33	0.74
1:E:556:ILE:CG2	1:E:557:SER:H	1.94	0.74
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.68	0.74
1:A:321:LYS:O	1:A:325:ARG:HG3	1.86	0.74
1:C:251:ASN:HB2	1:C:254:THR:OG1	1.88	0.74
1:C:584:ASN:HD21	1:C:694:HIS:H	1.32	0.74
1:E:546:GLU:HG3	1:E:547:HIS:CD2	2.23	0.74
1:C:494:GLU:O	1:C:555:LYS:HB3	1.87	0.74
1:A:235:VAL:HG21	1:A:240:MET:HB2	1.69	0.74
1:C:810:ASP:OD1	1:C:812:THR:HG22	1.88	0.74
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.70	0.74
1:A:132:ILE:HD12	1:A:162:ARG:HD3	1.70	0.74
1:C:316:GLY:N	1:C:319:LEU:HB2	2.02	0.74
1:C:533:THR:H	1:C:537:HIS:CD2	2.05	0.74
1:C:611:ASP:OD2	1:C:613:LYS:HB2	1.88	0.74
2:D:427:ARG:O	2:D:431:GLU:HG3	1.86	0.74
1:A:500:ASP:CB	1:A:552:VAL:HG11	2.18	0.73
1:E:734:GLN:N	1:E:734:GLN:HE21	1.86	0.73
1:E:26:ALA:CB	1:E:128:VAL:HB	2.17	0.73
1:A:561:VAL:HG21	1:A:775:ASN:HA	1.68	0.73
1:A:836:GLN:H	1:A:836:GLN:HE21	1.34	0.73
2:B:495:ASN:N	2:B:495:ASN:HD22	1.84	0.73
1:C:2:VAL:HG22	1:C:3:ALA:N	2.02	0.73
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.04	0.73
2:F:487:PRO:HA	2:F:492:ARG:O	1.89	0.73
2:B:427:ARG:O	2:B:431:GLU:HG3	1.88	0.73
1:E:500:ASP:OD2	1:E:552:VAL:HG21	1.87	0.73
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.71	0.72
1:C:501:LEU:C	1:C:501:LEU:HD23	2.14	0.72
1:C:523:SER:OG	1:C:527:GLU:HB2	1.88	0.72
1:E:74:ALA:O	1:E:439:GLY:HA2	1.89	0.72
1:A:584:ASN:HD21	1:A:694:HIS:H	1.37	0.72
2:B:477:LEU:HD13	2:B:551:ARG:NH1	2.03	0.72
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.72	0.72
1:C:243:ARG:NH1	1:C:257:TRP:CG	2.57	0.72
1:A:581:ASN:ND2	1:A:704:GLN:HG3	2.03	0.72
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.19	0.72
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.72	0.72
1:C:25:ILE:HD12	1:C:125:ALA:HB1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:THR:OG1	1:E:389:SER:HB3	1.90	0.72
1:A:627:VAL:CG1	2:F:405:GLY:HA2	2.20	0.71
1:E:236:ASP:OD1	1:E:238:ALA:HB3	1.90	0.71
1:E:581:ASN:ND2	1:E:704:GLN:HG3	2.05	0.71
1:A:27:HIS:CD2	1:A:29:ASP:H	2.09	0.71
1:A:588:LEU:HD12	1:A:588:LEU:C	2.15	0.71
2:B:455:VAL:O	2:B:456:ARG:HD2	1.91	0.71
1:C:828:MET:HE2	2:D:576:ARG:HE	1.55	0.71
1:E:87:LYS:HA	1:E:87:LYS:CE	2.20	0.71
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.72	0.71
1:C:454:ILE:HG13	1:C:455:GLY:H	1.54	0.71
1:C:166:GLU:C	1:C:167:LEU:HD12	2.14	0.71
1:C:694:HIS:O	1:C:700:ARG:HD3	1.91	0.71
1:A:32:LYS:NZ	1:A:105:SER:HB2	2.06	0.71
1:C:171:LYS:HG2	1:C:282:PHE:CD1	2.25	0.71
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.72	0.71
1:C:183:GLU:O	1:C:187:VAL:HG23	1.90	0.71
1:A:681:MET:HE2	1:A:717:PHE:CD1	2.26	0.70
1:E:552:VAL:CG2	1:E:553:PRO:HD3	2.19	0.70
1:E:828:MET:HE2	2:F:576:ARG:HE	1.55	0.70
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.71	0.70
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.73	0.70
1:E:503:LYS:HB3	1:E:551:GLY:CA	2.22	0.70
1:C:158:ASN:ND2	1:C:159:LYS:HG2	2.06	0.70
1:C:484:SER:HB3	1:C:797:VAL:CG2	2.21	0.70
1:E:338:ILE:O	1:E:342:LEU:HB2	1.92	0.70
2:D:556:LEU:HD22	2:D:560:LEU:HD13	1.74	0.70
1:A:25:ILE:HD12	1:A:125:ALA:HB1	1.74	0.69
1:A:607:ASN:OD1	1:A:609:ARG:HG3	1.91	0.69
1:A:410:LYS:HA	1:A:430:ALA:HA	1.73	0.69
1:E:87:LYS:HA	1:E:87:LYS:HE2	1.73	0.69
1:C:263:ASP:O	1:C:265:GLU:N	2.25	0.69
1:E:331:ALA:O	1:E:335:LEU:HG	1.92	0.69
1:C:584:ASN:ND2	1:C:694:HIS:H	1.90	0.69
1:C:694:HIS:CD2	1:C:696:ASP:H	2.08	0.69
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.74	0.69
1:A:35:LEU:HD22	1:A:334:LEU:HD11	1.75	0.69
1:E:238:ALA:HA	1:E:241:MET:HE3	1.75	0.69
2:D:477:LEU:HB2	2:D:551:ARG:HD2	1.75	0.69
1:E:496:LYS:HD3	1:E:555:LYS:HE2	1.74	0.69
1:A:615:ARG:HG2	1:A:619:MET:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.74	0.69
1:C:166:GLU:HB3	1:C:167:LEU:HD12	1.73	0.69
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.74	0.69
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.75	0.69
1:A:565:GLU:HG2	1:A:676:ILE:HD12	1.75	0.69
1:E:607:ASN:HB3	1:E:610:ASP:OD2	1.93	0.69
1:C:588:LEU:C	1:C:588:LEU:HD12	2.18	0.68
1:E:737:GLU:HG3	1:E:766:PHE:CE1	2.28	0.68
1:E:141:THR:HA	1:E:144:ARG:NH2	2.08	0.68
1:A:433:ARG:HH21	1:A:444:PRO:HB3	1.58	0.68
1:E:185:VAL:O	1:E:189:VAL:HG23	1.93	0.68
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.32	0.68
1:A:277:ILE:O	1:A:280:PRO:HD2	1.93	0.68
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.76	0.68
1:C:253:LYS:HE3	1:C:253:LYS:CA	2.20	0.68
1:C:506:GLU:HG3	1:C:510:ARG:CZ	2.23	0.68
1:C:117:ALA:N	1:C:481:MET:HE1	2.07	0.68
1:C:533:THR:H	1:C:537:HIS:HD2	1.42	0.68
1:C:734:GLN:N	1:C:734:GLN:HE21	1.92	0.68
1:E:496:LYS:HB2	1:E:555:LYS:HZ3	1.59	0.68
1:A:260:LYS:HE3	1:A:262:THR:O	1.93	0.67
1:A:459:ILE:HG21	1:A:463:LEU:HD12	1.76	0.67
1:C:10:ARG:HD3	1:C:445:ILE:HD11	1.76	0.67
1:E:836:GLN:H	1:E:836:GLN:NE2	1.91	0.67
1:A:836:GLN:H	1:A:836:GLN:NE2	1.92	0.67
1:E:186:ASN:CG	1:E:201:GLN:HE21	2.03	0.67
1:E:578:LYS:HE2	1:E:840:ASP:OD1	1.95	0.67
2:F:552:LEU:HD12	2:F:552:LEU:N	2.09	0.67
1:A:169:VAL:HG22	1:A:173:ASP:HB2	1.76	0.67
1:C:189:VAL:CG1	1:C:200:VAL:HG12	2.24	0.67
1:E:75:ILE:HD13	1:E:439:GLY:CA	2.24	0.67
1:E:589:LYS:HE3	1:E:689:LEU:HD11	1.76	0.67
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.76	0.67
1:A:132:ILE:CD1	1:A:162:ARG:HD3	2.25	0.67
1:A:591:GLU:O	1:A:685:ARG:HB3	1.94	0.67
1:E:588:LEU:C	1:E:588:LEU:HD12	2.19	0.67
1:C:110:ASP:OD1	1:C:781:THR:HG21	1.95	0.67
1:E:709:MET:HE3	1:E:713:THR:OG1	1.95	0.67
1:E:836:GLN:H	1:E:836:GLN:HE21	1.42	0.66
1:C:103:ILE:HD11	1:C:453:ILE:HG12	1.78	0.66
2:B:467:ARG:HG3	2:B:558:TRP:CD1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:GLU:O	1:C:539:GLU:HG3	1.95	0.66
1:C:45:ILE:HD11	1:C:78:TYR:CB	2.25	0.66
2:D:486:GLU:OE1	2:D:487:PRO:HD2	1.95	0.66
1:E:91:GLN:NE2	1:E:344:SER:H	1.92	0.66
1:A:584:ASN:ND2	1:A:694:HIS:H	1.93	0.66
1:C:192:TYR:HA	1:C:763:THR:HG21	1.78	0.66
1:C:315:GLU:CA	1:C:319:LEU:HB2	2.25	0.66
1:C:109:VAL:HG13	1:C:793:PHE:HE1	1.59	0.66
1:C:234:GLY:O	1:C:235:VAL:HG23	1.95	0.66
1:C:256:LYS:HA	1:C:256:LYS:CE	2.25	0.66
1:C:565:GLU:O	1:C:681:MET:HA	1.95	0.66
1:E:226:ALA:O	1:E:230:ALA:HB2	1.96	0.66
1:E:321:LYS:O	1:E:325:ARG:HG3	1.95	0.66
1:E:565:GLU:O	1:E:681:MET:HA	1.96	0.66
1:A:288:ILE:HG23	1:A:319:LEU:HD23	1.77	0.66
1:C:320:LEU:HD12	1:C:324:MET:HG3	1.77	0.66
1:E:142:VAL:O	1:E:145:GLN:HB2	1.96	0.66
1:A:392:GLY:HA2	1:A:513:LYS:HE2	1.76	0.66
2:B:417:TRP:NE1	2:B:568:PRO:HB2	2.10	0.66
1:E:584:ASN:ND2	1:E:694:HIS:H	1.93	0.66
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.77	0.65
1:E:89:ILE:C	1:E:91:GLN:H	2.03	0.65
1:A:644:ASN:HD22	1:A:684:VAL:HB	1.62	0.65
1:E:87:LYS:HE2	1:E:87:LYS:CA	2.26	0.65
1:E:654:GLN:HG2	1:E:655:TYR:CD2	2.31	0.65
2:F:465:ILE:HD12	2:F:535:LEU:HD12	1.77	0.65
1:A:581:ASN:ND2	1:A:699:DDE:O	2.28	0.65
1:C:162:ARG:HD2	1:C:166:GLU:OE2	1.97	0.65
1:C:703:GLY:HA2	2:D:493:ILE:HD13	1.78	0.65
1:E:536:LEU:HD11	1:E:540:ILE:HD11	1.77	0.65
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.78	0.65
1:E:279:ASP:O	1:E:283:ARG:HG2	1.97	0.65
1:A:258:THR:HG22	1:A:259:ASN:N	2.12	0.65
2:B:490:ARG:HD2	2:B:490:ARG:N	2.12	0.65
2:B:537:LEU:O	2:B:538:ARG:HD3	1.96	0.65
1:C:284:LEU:O	1:C:288:ILE:HB	1.97	0.65
1:E:292:LYS:HD3	1:E:295:GLU:OE2	1.96	0.64
1:A:220:PHE:HB3	1:A:328:LEU:HD13	1.78	0.64
1:C:243:ARG:NH1	1:C:257:TRP:CD1	2.65	0.64
1:A:373:ASP:OD2	1:A:376:ALA:HB2	1.98	0.64
1:E:211:PHE:HD2	1:E:220:PHE:CE1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:ARG:HE	1:C:687:ASN:HD21	1.46	0.64
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.78	0.64
1:A:7:ASP:HA	1:A:10:ARG:HG2	1.79	0.64
1:A:103:ILE:HD11	1:A:453:ILE:HG12	1.80	0.64
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.78	0.64
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.80	0.64
1:C:166:GLU:HB3	1:C:167:LEU:CD1	2.28	0.64
1:C:509:LYS:N	1:C:509:LYS:HD2	2.11	0.64
1:C:545:LEU:O	1:C:550:ALA:CB	2.45	0.64
1:E:736:PRO:HB2	1:E:738:GLN:HG2	1.78	0.64
1:C:285:PHE:HE2	1:C:324:MET:SD	2.21	0.64
1:C:491:VAL:O	1:C:529:ILE:HA	1.97	0.64
1:C:492:ALA:HA	1:C:528:HIS:O	1.97	0.64
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.63	0.63
1:E:584:ASN:HD21	1:E:694:HIS:H	1.45	0.63
1:A:348:ALA:HA	1:A:351:TYR:CE2	2.33	0.63
1:C:157:ILE:HD12	1:C:181:THR:HG21	1.79	0.63
1:C:316:GLY:N	1:C:319:LEU:CB	2.61	0.63
1:C:757:GLU:HG3	1:C:768:VAL:HG22	1.79	0.63
1:C:192:TYR:HA	1:C:763:THR:CG2	2.29	0.63
1:A:580:PRO:O	1:A:582:LYS:HG2	1.99	0.63
1:C:410:LYS:HA	1:C:430:ALA:HA	1.81	0.63
1:C:239:LYS:O	1:C:243:ARG:HG3	1.99	0.63
1:A:222:ILE:HG22	1:A:241:MET:HB2	1.80	0.63
1:A:454:ILE:HG13	1:A:455:GLY:N	2.11	0.63
1:C:38:SER:HA	1:C:41:GLN:HG2	1.80	0.63
1:C:581:ASN:O	1:C:582:LYS:HB2	1.98	0.63
1:A:589:LYS:HE3	1:A:689:LEU:HD11	1.80	0.63
1:E:166:GLU:HB3	1:E:167:LEU:HD12	1.81	0.63
1:A:719:LEU:HD21	1:A:835:TRP:CD2	2.35	0.62
1:C:220:PHE:HA	1:C:224:GLN:OE1	1.98	0.62
1:A:251:ASN:HB3	1:A:254:THR:OG1	1.99	0.62
2:B:524:ALA:O	2:B:528:GLU:HG3	1.99	0.62
1:E:75:ILE:HD13	1:E:439:GLY:HA3	1.81	0.62
1:E:495:VAL:CG1	1:E:554:LEU:HD23	2.28	0.62
1:A:568:GLU:HB3	1:A:721:ASP:OD2	1.99	0.62
1:C:256:LYS:HD3	1:C:257:TRP:N	2.11	0.62
1:E:704:GLN:O	1:E:707:PRO:HD2	1.99	0.62
1:E:275:MET:HE2	1:E:276:PHE:CE1	2.35	0.62
1:C:157:ILE:HD11	1:C:181:THR:HG21	1.82	0.62
1:C:615:ARG:HG2	1:C:619:MET:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:LYS:HE3	1:C:232:LYS:CG	2.23	0.62
1:C:277:ILE:O	1:C:280:PRO:HD2	1.99	0.62
1:E:307:LEU:HD13	1:E:312:LYS:HA	1.82	0.62
2:B:551:ARG:HG3	2:B:551:ARG:HH11	1.65	0.62
1:C:401:PHE:CD2	1:C:478:MET:HE1	2.35	0.62
1:C:784:LEU:HD23	1:C:794:PRO:CG	2.26	0.62
1:E:635:CYS:SG	1:E:664:VAL:HG13	2.40	0.62
1:A:581:ASN:HD21	1:A:704:GLN:HG3	1.64	0.62
1:A:694:HIS:CD2	1:A:696:ASP:H	2.09	0.62
1:C:522:MET:HA	1:C:527:GLU:O	2.00	0.62
1:E:311:GLU:HB3	1:E:322:VAL:HG11	1.82	0.62
2:F:524:ALA:O	2:F:528:GLU:HG3	1.98	0.62
1:A:183:GLU:O	1:A:187:VAL:HG23	1.99	0.61
1:A:647:ILE:HG13	1:A:685:ARG:NE	2.13	0.61
1:A:828:MET:HE2	2:B:576:ARG:NE	2.14	0.61
2:B:440:HIS:HB2	2:B:471:ILE:HG22	1.82	0.61
1:A:2:VAL:HG22	1:A:3:ALA:N	2.14	0.61
1:A:32:LYS:HZ3	1:A:105:SER:HB2	1.63	0.61
2:B:495:ASN:ND2	2:B:495:ASN:H	1.97	0.61
1:E:285:PHE:CE2	1:E:320:LEU:HD11	2.35	0.61
1:A:321:LYS:NZ	1:A:325:ARG:HD3	2.15	0.61
1:A:591:GLU:HG2	1:A:685:ARG:HG2	1.81	0.61
1:C:4:PHE:HD1	1:C:8:GLN:OE1	1.83	0.61
1:C:354:GLU:OE2	1:C:361:ALA:HB1	2.00	0.61
1:E:496:LYS:HD3	1:E:555:LYS:CE	2.30	0.61
1:C:348:ALA:HA	1:C:351:TYR:CE2	2.35	0.61
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.80	0.61
1:C:275:MET:HE2	1:C:276:PHE:CE1	2.36	0.61
1:E:91:GLN:HE22	1:E:344:SER:N	1.94	0.61
1:E:203:TYR:HD2	1:E:206:ARG:HD2	1.64	0.61
1:A:391:LYS:HG3	1:A:392:GLY:H	1.65	0.61
1:C:316:GLY:H	1:C:319:LEU:HB2	1.64	0.61
1:E:132:ILE:HD12	1:E:132:ILE:N	2.15	0.61
1:C:72:SER:HA	1:C:439:GLY:O	2.00	0.61
1:C:288:ILE:HG23	1:C:319:LEU:CD2	2.31	0.61
1:E:759:GLN:HB2	1:E:766:PHE:CE2	2.35	0.61
1:A:30:HIS:HA	1:A:159:LYS:CE	2.31	0.61
1:A:186:ASN:HB3	1:A:201:GLN:HG2	1.81	0.61
1:E:591:GLU:O	1:E:685:ARG:HB3	2.01	0.61
1:A:594:ASP:HB2	1:A:597:VAL:HG23	1.83	0.61
2:D:417:TRP:NE1	2:D:568:PRO:HB2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.65	0.61
1:A:411:VAL:HG12	1:A:412:ARG:N	2.15	0.60
1:C:5:THR:OG1	1:C:8:GLN:HG3	2.00	0.60
1:E:552:VAL:HG22	1:E:553:PRO:HD2	1.82	0.60
2:B:457:ALA:HB2	2:B:558:TRP:CD2	2.36	0.60
1:E:412:ARG:HH12	1:E:428:ILE:HD11	1.66	0.60
1:C:707:PRO:O	1:C:711:ARG:HG3	2.00	0.60
1:E:211:PHE:CD2	1:E:220:PHE:CE1	2.89	0.60
1:E:536:LEU:O	1:E:539:GLU:N	2.34	0.60
1:A:823:ARG:NH1	1:A:829:LYS:O	2.34	0.60
1:A:501:LEU:HB3	1:A:502:PRO:HD3	1.84	0.60
1:A:485:VAL:O	1:A:487:PRO:HD3	2.01	0.60
1:C:221:THR:OG1	1:C:224:GLN:HG3	2.01	0.60
1:E:69:THR:O	1:E:389:SER:N	2.34	0.60
1:E:728:VAL:HB	1:E:800:HIS:CD2	2.36	0.60
1:C:607:ASN:HB3	1:C:610:ASP:CG	2.26	0.60
1:E:381:TYR:O	1:E:398:GLY:HA3	2.01	0.60
1:A:186:ASN:HB3	1:A:201:GLN:HE21	1.67	0.60
1:C:216:HIS:CE1	1:C:317:LYS:HZ1	2.20	0.60
1:C:591:GLU:CG	1:C:685:ARG:HG2	2.32	0.60
1:E:43:ALA:HB1	1:E:78:TYR:O	2.02	0.60
1:E:126:LEU:HD11	1:E:156:VAL:CG2	2.32	0.60
1:A:172:GLU:OE2	1:A:271:ARG:NH2	2.35	0.60
1:A:459:ILE:HD11	1:A:469:LEU:HD21	1.84	0.60
1:C:3:ALA:HA	1:C:46:ILE:O	2.02	0.60
1:C:171:LYS:HG2	1:C:282:PHE:CE1	2.37	0.60
1:C:384:LYS:HB2	1:C:465:LYS:NZ	2.16	0.60
1:E:221:THR:OG1	1:E:224:GLN:HG3	2.02	0.60
1:C:500:ASP:OD2	1:C:552:VAL:HG21	2.02	0.59
2:D:477:LEU:HD13	2:D:551:ARG:NH1	2.17	0.59
2:D:551:ARG:HG3	2:D:551:ARG:HH11	1.67	0.59
1:A:690:ASP:OD1	1:A:691:VAL:N	2.30	0.59
1:A:544:ASP:O	1:A:549:HIS:HD2	1.85	0.59
1:C:581:ASN:ND2	1:C:699:DDE:O	2.35	0.59
1:C:581:ASN:HB3	1:C:583:HIS:HB2	1.84	0.59
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.84	0.59
2:F:420:GLU:CD	2:F:420:GLU:H	2.10	0.59
1:A:258:THR:HG22	1:A:259:ASN:H	1.67	0.59
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.84	0.59
1:E:303:LEU:O	1:E:304:GLU:HB2	2.03	0.59
2:D:455:VAL:O	2:D:456:ARG:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:LYS:O	1:E:386:VAL:HG21	2.03	0.59
1:E:176:GLN:O	1:E:180:ARG:HG3	2.02	0.59
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.84	0.59
1:A:591:GLU:CG	1:A:685:ARG:HG2	2.32	0.59
1:C:316:GLY:H	1:C:319:LEU:CB	2.15	0.59
1:C:404:THR:HG22	1:C:449:PRO:CA	2.27	0.59
1:C:685:ARG:NE	1:C:687:ASN:HD21	1.99	0.59
1:C:784:LEU:CD2	1:C:794:PRO:HG3	2.26	0.59
1:E:381:TYR:OH	1:E:481:MET:HE2	2.03	0.59
1:E:690:ASP:OD1	1:E:691:VAL:N	2.35	0.59
1:C:644:ASN:ND2	1:C:684:VAL:H	2.00	0.59
1:E:10:ARG:NH1	1:E:449:PRO:HD3	2.16	0.59
1:E:581:ASN:O	1:E:582:LYS:HB2	2.01	0.59
1:A:258:THR:HG22	1:A:260:LYS:H	1.67	0.59
1:A:381:TYR:O	1:A:398:GLY:HA3	2.02	0.59
1:C:497:ASN:N	1:C:497:ASN:ND2	2.50	0.59
2:B:551:ARG:NH1	2:B:551:ARG:HG3	2.17	0.59
1:C:35:LEU:HD22	1:C:334:LEU:HD11	1.84	0.59
1:E:255:LYS:O	1:E:256:LYS:HG2	2.03	0.59
1:E:410:LYS:HA	1:E:430:ALA:HA	1.84	0.59
1:A:30:HIS:HA	1:A:159:LYS:HE3	1.84	0.58
1:C:454:ILE:HG13	1:C:455:GLY:N	2.18	0.58
1:E:183:GLU:OE1	1:E:186:ASN:ND2	2.36	0.58
1:A:321:LYS:HZ2	1:A:325:ARG:HD3	1.68	0.58
2:B:420:GLU:OE1	2:B:420:GLU:N	2.35	0.58
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.18	0.58
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.85	0.58
1:A:406:LYS:O	1:A:409:GLN:HB3	2.01	0.58
1:A:501:LEU:C	1:A:501:LEU:HD23	2.29	0.58
1:E:258:THR:HG22	1:E:259:ASN:H	1.68	0.58
1:C:226:ALA:O	1:C:230:ALA:HB2	2.04	0.58
1:C:614:ALA:O	1:C:618:ILE:HG12	2.03	0.58
1:A:447:ASP:CG	1:A:448:CYS:N	2.61	0.58
1:C:258:THR:HG22	1:C:259:ASN:N	2.18	0.58
1:C:314:LEU:HD21	1:C:318:ALA:O	2.03	0.58
1:C:654:GLN:HG2	1:C:655:TYR:CD2	2.38	0.58
1:A:520:THR:HA	1:A:529:ILE:O	2.03	0.58
1:A:758:GLU:O	1:A:766:PHE:HD1	1.86	0.58
1:A:763:THR:HB	1:A:764:PRO:HD2	1.84	0.58
2:B:477:LEU:HD22	2:B:551:ARG:HB2	1.86	0.58
1:C:9:MET:O	1:C:13:MET:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.86	0.58
1:E:478:MET:O	1:E:479:LYS:C	2.47	0.58
1:A:828:MET:HE2	2:B:576:ARG:HE	1.69	0.57
1:C:236:ASP:OD2	1:C:239:LYS:HE2	2.04	0.57
1:E:391:LYS:HG3	1:E:392:GLY:H	1.69	0.57
1:A:385:MET:HE2	1:A:460:ASP:HA	1.85	0.57
1:A:561:VAL:HG21	1:A:775:ASN:CA	2.34	0.57
1:C:529:ILE:N	1:C:529:ILE:HD12	2.19	0.57
2:F:520:ALA:HB1	2:F:522:GLU:OE2	2.05	0.57
1:E:145:GLN:NE2	1:E:793:PHE:CZ	2.72	0.57
1:E:685:ARG:HE	1:E:687:ASN:HD21	1.53	0.57
2:F:488:ASP:CG	2:F:492:ARG:HB2	2.28	0.57
1:E:126:LEU:HD11	1:E:156:VAL:HG21	1.86	0.57
1:C:414:GLN:HB3	1:C:418:TYR:CD2	2.39	0.57
1:E:284:LEU:HD13	1:E:324:MET:HE1	1.84	0.57
1:E:412:ARG:HH11	1:E:412:ARG:HG2	1.69	0.57
2:F:433:GLY:O	2:F:505:ARG:HB2	2.04	0.57
1:A:7:ASP:O	1:A:10:ARG:HG2	2.05	0.57
1:A:132:ILE:HD12	1:A:162:ARG:HD2	1.84	0.57
1:A:493:VAL:HG12	1:A:554:LEU:HD22	1.86	0.57
1:E:561:VAL:HG21	1:E:775:ASN:CB	2.34	0.57
2:D:445:GLU:OE1	2:D:494:ARG:NH2	2.38	0.57
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.86	0.57
1:C:644:ASN:HD22	1:C:684:VAL:H	1.53	0.57
1:E:365:ASN:O	1:E:369:ILE:HG12	2.05	0.57
1:E:556:ILE:N	1:E:556:ILE:HD12	2.20	0.57
1:E:736:PRO:HB2	1:E:738:GLN:CG	2.35	0.57
1:C:251:ASN:OD1	1:C:269:LEU:HD11	2.05	0.57
1:C:509:LYS:O	1:C:513:LYS:HE3	2.05	0.57
1:E:591:GLU:CG	1:E:685:ARG:HG2	2.35	0.57
1:C:231:LYS:HG2	1:C:232:LYS:N	2.19	0.56
1:C:546:GLU:HG3	1:C:553:PRO:HA	1.87	0.56
1:C:627:VAL:HG21	1:C:631:ARG:NH2	2.20	0.56
1:E:258:THR:HG22	1:E:259:ASN:N	2.20	0.56
2:F:522:GLU:CD	2:F:522:GLU:H	2.12	0.56
1:A:521:TYR:CE1	1:A:529:ILE:HD12	2.40	0.56
1:C:732:GLU:OE1	1:C:769:LYS:HE3	2.04	0.56
1:A:478:MET:O	1:A:479:LYS:C	2.48	0.56
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.87	0.56
1:C:493:VAL:HG21	1:C:545:LEU:HD21	1.86	0.56
1:C:497:ASN:N	1:C:497:ASN:HD22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:ASP:HB2	1:C:597:VAL:HG23	1.87	0.56
2:D:438:GLY:HA3	2:D:471:ILE:HD12	1.86	0.56
1:E:71:LYS:HB3	1:E:386:VAL:CG2	2.33	0.56
1:E:749:LYS:O	1:E:750:LYS:HD2	2.05	0.56
1:A:156:VAL:HG21	1:A:334:LEU:CD2	2.35	0.56
1:A:156:VAL:HG21	1:A:334:LEU:HD22	1.88	0.56
1:A:172:GLU:CD	1:A:271:ARG:HH21	2.13	0.56
1:A:647:ILE:HB	1:A:687:ASN:HD22	1.70	0.56
2:B:484:ASP:OD2	2:B:494:ARG:HG2	2.05	0.56
1:C:155:VAL:HG12	1:C:156:VAL:N	2.19	0.56
1:C:251:ASN:H	1:C:251:ASN:HD22	1.54	0.56
1:C:494:GLU:OE1	1:C:494:GLU:HA	2.04	0.56
1:C:550:ALA:O	1:C:552:VAL:N	2.38	0.56
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.86	0.56
1:E:722:PRO:O	1:E:723:LYS:HD2	2.04	0.56
1:A:162:ARG:O	1:A:166:GLU:HB2	2.06	0.56
1:A:550:ALA:O	1:A:552:VAL:HG23	2.05	0.56
2:F:488:ASP:OD2	2:F:492:ARG:HD3	2.05	0.56
1:A:111:PHE:HB3	1:A:114:GLU:HG2	1.87	0.56
1:C:524:GLU:C	1:C:526:GLY:H	2.14	0.56
2:D:432:ARG:CZ	2:D:432:ARG:HA	2.35	0.56
1:E:37:ASP:O	1:E:41:GLN:HG3	2.05	0.56
1:A:734:GLN:HE21	1:A:734:GLN:N	2.04	0.56
1:E:225:PHE:CD2	1:E:277:ILE:HD12	2.41	0.56
1:E:158:ASN:HD22	1:E:159:LYS:HG3	1.70	0.56
1:E:186:ASN:OD1	1:E:186:ASN:C	2.49	0.56
2:F:473:GLY:HA3	2:F:597:LEU:HD11	1.88	0.56
2:B:405:GLY:HA2	1:C:627:VAL:HG12	1.88	0.56
1:C:240:MET:O	1:C:244:LEU:HG	2.05	0.56
1:C:484:SER:HB3	1:C:797:VAL:HG22	1.88	0.56
1:E:240:MET:O	1:E:244:LEU:HG	2.05	0.56
1:C:42:ARG:HG3	1:C:331:ALA:HB3	1.85	0.56
1:A:220:PHE:HA	1:A:224:GLN:OE1	2.04	0.55
1:C:538:LEU:O	1:C:542:LEU:HG	2.06	0.55
1:A:486:SER:O	1:A:488:VAL:HG13	2.05	0.55
1:E:114:GLU:O	1:E:117:ALA:HB3	2.06	0.55
1:E:250:PHE:HD2	1:E:275:MET:HE1	1.70	0.55
1:E:432:GLN:HB2	1:E:457:VAL:O	2.06	0.55
1:E:707:PRO:O	1:E:711:ARG:HG3	2.06	0.55
1:A:110:ASP:C	1:A:112:SER:H	2.14	0.55
1:A:155:VAL:O	1:A:337:MET:HE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.70	0.55
2:B:495:ASN:N	2:B:495:ASN:ND2	2.47	0.55
1:E:150:ARG:CZ	1:E:355:GLN:OE1	2.55	0.55
1:C:27:HIS:CD2	1:C:29:ASP:H	2.20	0.55
1:E:26:ALA:O	1:E:32:LYS:HD2	2.06	0.55
1:A:140:GLU:HG3	1:A:188:ILE:HD11	1.85	0.55
1:A:231:LYS:C	1:A:233:PHE:H	2.15	0.55
2:B:495:ASN:HD22	2:B:495:ASN:H	1.53	0.55
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.88	0.55
1:C:675:PRO:HD3	1:C:714:TYR:CE1	2.41	0.55
1:A:3:ALA:HA	1:A:46:ILE:O	2.07	0.55
1:A:4:PHE:HA	1:A:8:GLN:OE1	2.07	0.55
1:A:229:TYR:HE2	1:A:276:PHE:HB3	1.68	0.55
1:A:820:LEU:CD1	1:A:830:GLU:HG2	2.34	0.55
2:B:518:LEU:HD22	2:B:518:LEU:H	1.72	0.55
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.89	0.55
1:C:563:TYR:O	1:C:564:ARG:HD2	2.07	0.55
1:C:585:ARG:HD2	1:C:692:THR:OG1	2.07	0.55
1:E:496:LYS:HD3	1:E:555:LYS:NZ	2.20	0.55
2:F:500:ARG:O	2:F:566:VAL:HG13	2.06	0.55
1:A:166:GLU:HB3	1:A:167:LEU:HD12	1.88	0.55
1:A:306:VAL:HG23	1:A:306:VAL:O	2.07	0.55
1:C:200:VAL:O	1:C:200:VAL:CG1	2.55	0.55
2:D:527:VAL:HG22	2:D:542:ILE:CD1	2.37	0.55
2:D:546:GLU:HG3	2:D:547:GLU:CG	2.33	0.55
1:E:9:MET:O	1:E:12:LEU:HB3	2.07	0.55
1:E:454:ILE:HG13	1:E:455:GLY:N	2.22	0.55
1:A:737:GLU:HG3	1:A:766:PHE:CD2	2.41	0.55
1:C:240:MET:O	1:C:240:MET:HE3	2.07	0.55
2:D:507:SER:C	2:D:509:PRO:HD2	2.32	0.55
1:E:179:ALA:O	1:E:183:GLU:HB2	2.07	0.55
1:E:225:PHE:CG	1:E:277:ILE:HD12	2.42	0.55
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.41	0.55
1:A:447:ASP:CG	1:A:448:CYS:H	2.15	0.54
1:C:25:ILE:CD1	1:C:125:ALA:HB1	2.37	0.54
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.88	0.54
1:C:669:TRP:NE1	1:C:710:ARG:HH21	2.06	0.54
1:E:167:LEU:HD12	1:E:167:LEU:H	1.71	0.54
2:F:467:ARG:HG3	2:F:558:TRP:CD1	2.43	0.54
1:A:155:VAL:HG12	1:A:156:VAL:N	2.21	0.54
1:A:223:ARG:HH11	1:A:223:ARG:HG2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:488:ASP:OD1	2:B:489:ALA:N	2.40	0.54
2:B:552:LEU:H	2:B:552:LEU:CD1	2.18	0.54
1:C:157:ILE:HD11	1:C:181:THR:CG2	2.37	0.54
1:C:288:ILE:HG23	1:C:319:LEU:HG	1.90	0.54
1:A:344:SER:C	1:A:346:VAL:H	2.15	0.54
1:A:581:ASN:C	1:A:582:LYS:CG	2.81	0.54
1:A:690:ASP:O	1:A:691:VAL:HG23	2.08	0.54
1:A:730:LEU:C	1:A:730:LEU:CD2	2.81	0.54
1:A:129:VAL:HG13	1:A:134:GLY:C	2.32	0.54
1:C:314:LEU:HG	1:C:319:LEU:HA	1.89	0.54
2:D:458:ARG:H	2:D:460:GLN:NE2	2.04	0.54
2:D:529:ARG:NH1	2:D:604:PRO:HG2	2.21	0.54
1:E:80:GLU:HA	1:E:96:ASN:O	2.06	0.54
1:E:348:ALA:O	1:E:352:ARG:HB2	2.06	0.54
1:E:669:TRP:CZ2	2:F:492:ARG:HG2	2.42	0.54
1:C:77:LEU:HB2	1:C:100:ILE:HB	1.88	0.54
1:C:288:ILE:HG23	1:C:319:LEU:CG	2.37	0.54
2:D:447:ALA:O	2:D:448:GLN:C	2.50	0.54
1:E:251:ASN:HB3	1:E:254:THR:OG1	2.07	0.54
1:A:737:GLU:CG	1:A:766:PHE:HE2	2.19	0.54
1:C:478:MET:O	1:C:479:LYS:C	2.50	0.54
1:E:68:ILE:HG23	1:E:390:ASP:HB2	1.90	0.54
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.89	0.54
1:C:126:LEU:HD11	1:C:156:VAL:CG2	2.37	0.54
1:C:490:GLN:O	1:C:491:VAL:HG13	2.07	0.54
1:C:584:ASN:ND2	1:C:693:LEU:HA	2.20	0.54
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.43	0.54
1:C:243:ARG:HH12	1:C:257:TRP:CD1	2.24	0.54
1:C:348:ALA:O	1:C:352:ARG:HB2	2.08	0.54
1:C:365:ASN:O	1:C:369:ILE:HG12	2.08	0.54
1:C:543:GLN:O	1:C:546:GLU:N	2.41	0.54
2:D:488:ASP:CG	2:D:489:ALA:N	2.66	0.54
1:E:278:LEU:O	1:E:282:PHE:HB2	2.08	0.54
1:A:466:THR:HG22	1:A:467:GLY:N	2.23	0.54
2:B:477:LEU:HD11	2:B:546:GLU:OE1	2.08	0.54
1:C:316:GLY:O	1:C:319:LEU:HB3	2.07	0.54
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.38	0.54
2:F:505:ARG:NH1	2:F:505:ARG:HG3	2.23	0.54
1:A:285:PHE:CE2	1:A:320:LEU:HD11	2.43	0.54
1:C:10:ARG:CZ	1:C:449:PRO:HD3	2.38	0.54
2:D:447:ALA:HA	2:D:499:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:CD1	1:A:469:LEU:HD21	2.37	0.53
1:A:669:TRP:CZ2	2:B:492:ARG:HB3	2.43	0.53
1:A:710:ARG:HG3	1:A:710:ARG:HH11	1.72	0.53
1:E:150:ARG:NH1	1:E:355:GLN:HB2	2.23	0.53
2:B:505:ARG:NH1	2:B:505:ARG:HG3	2.22	0.53
1:C:45:ILE:HD11	1:C:78:TYR:N	2.24	0.53
1:C:311:GLU:OE2	1:C:322:VAL:HG11	2.09	0.53
1:C:836:GLN:HE21	1:C:836:GLN:N	1.98	0.53
1:E:739:ALA:HB2	1:E:791:GLN:OE1	2.07	0.53
2:F:529:ARG:NH1	2:F:604:PRO:HG2	2.24	0.53
2:F:530:LEU:HA	2:F:604:PRO:HG3	1.89	0.53
1:E:75:ILE:HD13	1:E:439:GLY:HA2	1.89	0.53
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.91	0.53
1:A:117:ALA:HA	1:A:481:MET:SD	2.48	0.53
2:B:445:GLU:OE1	2:B:494:ARG:NH2	2.37	0.53
1:C:109:VAL:HG13	1:C:793:PHE:CE1	2.42	0.53
1:C:200:VAL:O	1:C:200:VAL:HG13	2.08	0.53
1:A:189:VAL:CG1	1:A:200:VAL:HG12	2.39	0.53
1:A:235:VAL:CG2	1:A:240:MET:HB2	2.39	0.53
1:C:466:THR:HG22	1:C:467:GLY:N	2.24	0.53
1:C:569:SER:O	1:C:720:ALA:HB1	2.08	0.53
1:E:289:MET:HE1	1:E:317:LYS:N	2.23	0.53
1:E:576:LEU:HD13	1:E:587:TYR:CE1	2.44	0.53
2:F:440:HIS:HB2	2:F:471:ILE:HG22	1.90	0.53
1:A:25:ILE:CD1	1:A:125:ALA:HB1	2.38	0.53
1:C:132:ILE:HG23	1:C:133:GLU:N	2.24	0.53
1:C:275:MET:HE2	1:C:276:PHE:CZ	2.42	0.53
1:A:472:SER:HB3	1:A:475:ALA:HB2	1.91	0.53
1:C:509:LYS:O	1:C:513:LYS:HG3	2.09	0.53
1:C:580:PRO:HD2	1:C:704:GLN:CD	2.34	0.53
1:C:782:GLY:O	1:C:785:ARG:HB3	2.09	0.53
2:D:551:ARG:NH1	2:D:551:ARG:HG3	2.23	0.53
2:D:457:ALA:HB2	2:D:558:TRP:CD2	2.44	0.53
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.34	0.53
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.44	0.53
1:C:45:ILE:HG12	1:C:76:SER:O	2.09	0.53
1:E:70:ILE:HG22	1:E:388:THR:HG22	1.89	0.53
1:A:200:VAL:O	1:A:200:VAL:HG13	2.07	0.53
1:C:132:ILE:HG23	1:C:133:GLU:HG3	1.91	0.53
1:C:344:SER:C	1:C:346:VAL:H	2.17	0.53
1:C:750:LYS:O	1:C:751:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:LYS:CD	1:E:200:VAL:HG23	2.38	0.53
1:E:307:LEU:HD12	1:E:312:LYS:HD3	1.91	0.53
1:C:129:VAL:HG13	1:C:134:GLY:O	2.09	0.52
1:C:429:LYS:HG3	1:C:462:PHE:CZ	2.43	0.52
1:E:9:MET:HE2	1:E:438:MET:SD	2.50	0.52
1:E:644:ASN:HD22	1:E:684:VAL:HB	1.74	0.52
1:C:291:PHE:HE1	1:C:315:GLU:HB2	1.74	0.52
1:C:468:THR:C	1:C:469:LEU:HD12	2.34	0.52
1:E:508:LEU:HD22	1:E:520:THR:HB	1.91	0.52
1:C:385:MET:HE2	1:C:460:ASP:HA	1.92	0.52
1:C:391:LYS:HD3	1:C:393:ARG:HG3	1.91	0.52
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.90	0.52
1:A:71:LYS:HB3	1:A:386:VAL:CG2	2.38	0.52
1:A:228:ARG:C	1:A:230:ALA:H	2.17	0.52
1:C:647:ILE:HG13	1:C:685:ARG:HE	1.73	0.52
1:C:647:ILE:HB	1:C:687:ASN:HD22	1.74	0.52
1:A:797:VAL:HG22	1:A:798:PHE:N	2.24	0.52
1:C:544:ASP:O	1:C:549:HIS:HB2	2.10	0.52
1:C:619:MET:HE1	1:C:633:ILE:CD1	2.39	0.52
1:E:17:THR:HB	1:E:92:LYS:O	2.09	0.52
1:C:243:ARG:HH11	1:C:257:TRP:CG	2.26	0.52
2:D:508:LEU:N	2:D:509:PRO:CD	2.73	0.52
1:E:289:MET:HE2	1:E:289:MET:HA	1.92	0.52
1:E:646:VAL:HG13	1:E:688:ILE:CD1	2.40	0.52
2:F:505:ARG:HG3	2:F:505:ARG:HH11	1.75	0.52
1:A:72:SER:HA	1:A:439:GLY:O	2.10	0.52
1:A:186:ASN:CB	1:A:201:GLN:HG2	2.40	0.52
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.91	0.52
1:C:155:VAL:CG1	1:C:156:VAL:N	2.72	0.52
1:C:436:LEU:HD23	1:C:454:ILE:CD1	2.40	0.52
1:E:171:LYS:NZ	1:E:283:ARG:NH2	2.57	0.52
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.92	0.52
1:C:126:LEU:HD11	1:C:156:VAL:HG21	1.92	0.52
1:C:258:THR:HG22	1:C:259:ASN:H	1.74	0.52
1:C:742:GLY:O	1:C:745:SER:HB3	2.10	0.52
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.45	0.52
2:B:429:LEU:HD21	2:B:565:VAL:HG11	1.91	0.52
1:C:384:LYS:HB2	1:C:465:LYS:HE3	1.92	0.52
1:C:743:ILE:HD13	1:C:784:LEU:HD11	1.91	0.52
1:E:103:ILE:HD12	1:E:103:ILE:N	2.23	0.52
1:E:493:VAL:HG12	1:E:494:GLU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:O	1:A:339:VAL:HG23	2.10	0.51
1:A:673:GLU:HG2	1:A:678:GLY:O	2.10	0.51
1:A:155:VAL:HG21	1:A:185:VAL:HG11	1.92	0.51
1:A:581:ASN:N	1:A:704:GLN:OE1	2.35	0.51
1:A:759:GLN:HB2	1:A:766:PHE:CE1	2.45	0.51
1:C:384:LYS:CB	1:C:465:LYS:HE3	2.40	0.51
1:E:13:MET:SD	1:E:436:LEU:HD21	2.50	0.51
1:A:493:VAL:CG1	1:A:554:LEU:HD22	2.40	0.51
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.38	0.51
2:F:426:HIS:NE2	2:F:594:ILE:HB	2.25	0.51
1:A:273:PHE:CD1	1:A:277:ILE:HD12	2.45	0.51
1:A:707:PRO:O	1:A:711:ARG:HG3	2.10	0.51
1:A:809:LEU:O	1:A:811:PRO:HD3	2.11	0.51
2:B:575:PRO:HG2	2:B:576:ARG:NH1	2.26	0.51
1:C:529:ILE:HG22	1:C:530:VAL:N	2.25	0.51
1:C:571:SER:HB2	1:C:589:LYS:HG2	1.91	0.51
1:E:229:TYR:CE2	1:E:276:PHE:HB3	2.45	0.51
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.91	0.51
1:C:226:ALA:CB	1:C:241:MET:HB3	2.41	0.51
1:C:335:LEU:O	1:C:339:VAL:HG23	2.10	0.51
1:E:387:PRO:HG3	1:E:394:PHE:CE1	2.45	0.51
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.45	0.51
1:E:500:ASP:O	1:E:503:LYS:HB2	2.10	0.51
1:E:528:HIS:C	1:E:529:ILE:HD13	2.35	0.51
2:B:460:GLN:HB3	2:B:467:ARG:HD3	1.92	0.51
1:C:544:ASP:O	1:C:549:HIS:N	2.44	0.51
1:E:385:MET:HE2	1:E:460:ASP:HA	1.93	0.51
1:E:750:LYS:O	1:E:751:ARG:HB2	2.10	0.51
1:A:155:VAL:CG1	1:A:156:VAL:N	2.74	0.51
2:B:420:GLU:N	2:B:420:GLU:CD	2.69	0.51
1:A:7:ASP:CA	1:A:10:ARG:HG2	2.40	0.51
1:A:9:MET:O	1:A:13:MET:HG3	2.11	0.51
1:A:401:PHE:CD2	1:A:478:MET:HE1	2.45	0.51
2:B:457:ALA:O	2:B:458:ARG:HG3	2.10	0.51
1:C:91:GLN:O	1:C:93:THR:HG23	2.10	0.51
1:C:265:GLU:CG	1:C:266:GLY:H	2.14	0.51
1:C:669:TRP:CD1	1:C:669:TRP:C	2.88	0.51
1:E:627:VAL:O	1:E:631:ARG:HG3	2.11	0.51
2:F:407:VAL:HG22	2:F:416:ASN:O	2.11	0.51
1:A:68:ILE:HG23	1:A:390:ASP:HB2	1.93	0.51
1:A:223:ARG:HG2	1:A:223:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:LEU:HB2	1:E:312:LYS:HE2	1.93	0.51
1:E:807:ASP:OD2	1:E:807:ASP:C	2.53	0.51
1:A:644:ASN:ND2	1:A:684:VAL:H	2.09	0.51
1:C:3:ALA:HA	1:C:46:ILE:HG22	1.93	0.50
1:C:208:THR:HG22	1:C:341:HIS:CG	2.46	0.50
1:C:262:THR:HA	1:C:269:LEU:HG	1.93	0.50
1:C:578:LYS:HA	1:C:584:ASN:O	2.11	0.50
1:E:10:ARG:HD3	1:E:445:ILE:HD11	1.92	0.50
1:E:43:ALA:O	1:E:77:LEU:HA	2.11	0.50
1:A:423:LYS:HG2	1:A:423:LYS:O	2.11	0.50
1:E:454:ILE:HG13	1:E:455:GLY:H	1.75	0.50
2:F:426:HIS:CE1	2:F:594:ILE:HB	2.46	0.50
1:A:581:ASN:O	1:A:582:LYS:HG3	2.11	0.50
1:C:619:MET:HE1	1:C:633:ILE:HD11	1.94	0.50
1:E:22:MET:HA	1:E:122:THR:HB	1.92	0.50
1:E:482:LYS:HB3	1:E:797:VAL:HG21	1.94	0.50
1:E:693:LEU:HB3	1:E:700:ARG:HD2	1.94	0.50
1:C:110:ASP:C	1:C:112:SER:H	2.20	0.50
1:C:132:ILE:HG23	1:C:133:GLU:H	1.77	0.50
2:D:546:GLU:HG2	2:D:547:GLU:HG3	1.91	0.50
2:D:552:LEU:N	2:D:552:LEU:HD12	2.27	0.50
1:E:809:LEU:O	1:E:811:PRO:HD3	2.12	0.50
1:A:226:ALA:CB	1:A:241:MET:HB3	2.41	0.50
1:A:406:LYS:HG3	1:A:409:GLN:HB2	1.94	0.50
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.47	0.50
1:A:709:MET:HE3	1:A:713:THR:OG1	2.12	0.50
2:B:508:LEU:N	2:B:509:PRO:CD	2.74	0.50
1:C:315:GLU:C	1:C:319:LEU:HB2	2.36	0.50
1:E:39:LEU:CD1	1:E:334:LEU:HD12	2.42	0.50
1:E:495:VAL:HA	1:E:554:LEU:HA	1.93	0.50
1:E:524:GLU:HA	2:F:492:ARG:HH12	1.76	0.50
1:A:7:ASP:HA	1:A:10:ARG:CG	2.42	0.50
1:A:29:ASP:O	1:A:159:LYS:NZ	2.29	0.50
1:A:485:VAL:O	1:A:485:VAL:HG22	2.12	0.50
1:C:129:VAL:HG12	1:C:130:ASP:N	2.27	0.50
1:C:709:MET:HE3	1:C:713:THR:OG1	2.12	0.50
2:D:484:ASP:OD2	2:D:494:ARG:HD3	2.12	0.50
2:D:524:ALA:O	2:D:528:GLU:HG3	2.11	0.50
1:E:597:VAL:O	1:E:601:ILE:HG13	2.11	0.50
1:A:3:ALA:HA	1:A:46:ILE:HG22	1.92	0.50
1:A:220:PHE:CD1	1:A:220:PHE:C	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:VAL:O	1:A:823:ARG:HG3	2.11	0.50
1:C:45:ILE:HG12	1:C:76:SER:C	2.36	0.50
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.47	0.50
2:F:426:HIS:O	2:F:429:LEU:HB2	2.11	0.50
2:F:513:ARG:HH11	2:F:513:ARG:CB	2.22	0.50
1:A:16:VAL:HG12	1:A:346:VAL:HG23	1.94	0.50
1:A:693:LEU:HB3	1:A:700:ARG:HD2	1.94	0.50
1:C:344:SER:C	1:C:346:VAL:N	2.70	0.50
1:C:506:GLU:HG3	1:C:510:ARG:HE	1.75	0.50
1:C:578:LYS:HG2	1:C:585:ARG:HG2	1.94	0.50
1:E:371:ASN:O	1:E:372:CYS:C	2.54	0.50
1:E:784:LEU:HD23	1:E:794:PRO:CG	2.38	0.50
1:A:153:PRO:HD2	1:A:200:VAL:HG13	1.94	0.50
1:A:388:THR:HG21	1:A:395:TYR:CG	2.46	0.50
1:C:106:PRO:HG3	1:C:114:GLU:HG3	1.93	0.50
1:C:167:LEU:HD12	1:C:167:LEU:N	2.25	0.50
1:C:627:VAL:O	1:C:631:ARG:HG3	2.12	0.50
1:E:39:LEU:HB3	1:E:77:LEU:HD21	1.92	0.50
1:E:39:LEU:HD11	1:E:334:LEU:CD1	2.42	0.50
1:E:235:VAL:HG11	1:E:239:LYS:HD3	1.94	0.50
1:A:411:VAL:CG1	1:A:412:ARG:N	2.74	0.49
2:B:420:GLU:CD	2:B:420:GLU:H	2.19	0.49
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.93	0.49
1:C:129:VAL:HG13	1:C:134:GLY:C	2.37	0.49
1:C:384:LYS:HB2	1:C:465:LYS:CE	2.42	0.49
1:C:601:ILE:HG12	1:C:606:ILE:HB	1.94	0.49
1:C:669:TRP:HE1	1:C:710:ARG:HH21	1.59	0.49
1:C:823:ARG:NH1	1:C:828:MET:HB2	2.26	0.49
1:E:563:TYR:O	1:E:564:ARG:HD2	2.12	0.49
1:E:585:ARG:HD2	1:E:692:THR:OG1	2.12	0.49
2:F:442:THR:OG1	2:F:443:PHE:N	2.42	0.49
1:A:584:ASN:ND2	1:A:693:LEU:HA	2.17	0.49
2:D:485:GLN:O	2:D:486:GLU:HG2	2.12	0.49
1:E:183:GLU:O	1:E:187:VAL:HG23	2.12	0.49
1:E:571:SER:HB2	1:E:589:LYS:HG2	1.93	0.49
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.94	0.49
1:A:132:ILE:HD12	1:A:162:ARG:NH1	2.22	0.49
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.47	0.49
2:B:410:SER:HB3	2:B:413:GLY:O	2.13	0.49
2:B:411:THR:OG1	2:B:495:ASN:ND2	2.43	0.49
1:E:581:ASN:HB3	1:E:583:HIS:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HG13	1:A:134:GLY:O	2.13	0.49
1:A:374:PRO:O	1:A:404:THR:HG23	2.12	0.49
1:C:228:ARG:C	1:C:230:ALA:H	2.20	0.49
1:E:754:VAL:HA	1:E:770:ALA:HB2	1.94	0.49
1:E:823:ARG:NH1	1:E:828:MET:HB2	2.27	0.49
1:C:2:VAL:CG2	1:C:3:ALA:H	2.19	0.49
2:D:558:TRP:O	2:D:559:PRO:C	2.55	0.49
1:E:296:ILE:O	1:E:300:LEU:HB2	2.12	0.49
1:E:650:THR:CG2	1:E:688:ILE:HG22	2.42	0.49
2:F:504:PRO:HD3	2:F:563:ARG:O	2.11	0.49
1:C:703:GLY:HA2	2:D:493:ILE:CD1	2.42	0.49
1:E:167:LEU:HD12	1:E:167:LEU:N	2.28	0.49
1:E:284:LEU:HD11	1:E:303:LEU:CD1	2.41	0.49
1:E:536:LEU:O	1:E:537:HIS:C	2.55	0.49
2:F:552:LEU:HD12	2:F:552:LEU:H	1.75	0.49
1:A:27:HIS:HD2	1:A:29:ASP:N	2.01	0.49
1:A:594:ASP:O	1:A:597:VAL:HG23	2.12	0.49
1:C:371:ASN:O	1:C:372:CYS:C	2.55	0.49
1:E:162:ARG:O	1:E:166:GLU:HB2	2.13	0.49
1:E:200:VAL:HG22	1:E:200:VAL:O	2.13	0.49
2:F:420:GLU:CD	2:F:420:GLU:N	2.71	0.49
2:F:451:VAL:O	2:F:451:VAL:CG1	2.59	0.49
1:C:729:PHE:CE2	1:C:774:VAL:HG22	2.47	0.49
2:D:548:GLU:O	2:D:548:GLU:HG3	2.11	0.49
1:A:191:THR:O	1:A:763:THR:HG22	2.13	0.49
1:A:231:LYS:C	1:A:233:PHE:N	2.70	0.49
2:B:453:GLY:O	2:B:456:ARG:HD3	2.12	0.49
1:C:148:GLY:HA2	1:C:760:ARG:NH2	2.28	0.49
1:C:729:PHE:O	1:C:771:TYR:HA	2.13	0.49
1:E:153:PRO:HD2	1:E:200:VAL:HG22	1.95	0.49
1:E:749:LYS:O	1:E:749:LYS:HG3	2.13	0.49
1:A:109:VAL:CG2	1:A:138:GLN:HG3	2.43	0.49
1:A:125:ALA:HB2	1:A:151:ILE:HG21	1.95	0.49
1:C:296:ILE:CD1	1:C:319:LEU:HD21	2.38	0.49
1:C:792:ALA:O	1:C:794:PRO:HD3	2.13	0.49
2:D:484:ASP:OD2	2:D:494:ARG:CD	2.60	0.49
1:E:109:VAL:HG23	1:E:138:GLN:CD	2.38	0.49
1:E:710:ARG:HG3	1:E:710:ARG:NH1	2.28	0.49
1:A:106:PRO:HG3	1:A:114:GLU:HG3	1.95	0.48
1:A:230:ALA:O	1:A:235:VAL:HG22	2.12	0.48
2:B:436:PHE:HB2	2:B:502:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.48	0.48
1:C:459:ILE:HG21	1:C:463:LEU:HD12	1.94	0.48
2:D:451:VAL:O	2:D:451:VAL:HG12	2.13	0.48
2:D:518:LEU:HD22	2:D:518:LEU:H	1.77	0.48
1:E:171:LYS:NZ	1:E:283:ARG:HH21	2.11	0.48
1:E:503:LYS:CB	1:E:551:GLY:HA3	2.38	0.48
1:A:175:TYR:HD2	1:A:176:GLN:HE21	1.61	0.48
1:C:390:ASP:O	1:C:391:LYS:HB3	2.13	0.48
1:C:607:ASN:HB3	1:C:610:ASP:OD2	2.13	0.48
1:E:374:PRO:O	1:E:404:THR:HG23	2.13	0.48
2:F:556:LEU:HD22	2:F:560:LEU:HD13	1.95	0.48
1:A:45:ILE:HB	1:A:76:SER:HB2	1.94	0.48
1:A:126:LEU:HD11	1:A:156:VAL:CG2	2.43	0.48
1:A:626:ASP:C	1:A:628:THR:N	2.71	0.48
2:B:551:ARG:HH11	2:B:551:ARG:CG	2.27	0.48
1:C:2:VAL:CG2	1:C:3:ALA:N	2.71	0.48
1:C:211:PHE:O	1:C:219:ALA:HA	2.13	0.48
1:E:606:ILE:HD12	1:E:619:MET:CG	2.43	0.48
2:F:427:ARG:HG2	2:F:428:GLN:N	2.28	0.48
1:A:77:LEU:HB2	1:A:100:ILE:HB	1.95	0.48
1:E:40:VAL:C	1:E:42:ARG:H	2.21	0.48
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.49	0.48
1:E:646:VAL:HG13	1:E:688:ILE:HD12	1.95	0.48
1:A:100:ILE:HD13	1:A:338:ILE:HG21	1.94	0.48
1:A:307:LEU:HD13	1:A:312:LYS:HA	1.96	0.48
1:A:504:LEU:HD13	1:A:554:LEU:HD21	1.96	0.48
1:C:314:LEU:CD2	1:C:318:ALA:O	2.61	0.48
1:C:712:ALA:O	1:C:715:ALA:HB3	2.13	0.48
1:E:186:ASN:HB2	1:E:201:GLN:HG2	1.96	0.48
1:A:2:VAL:CG2	1:A:3:ALA:N	2.77	0.48
1:A:588:LEU:C	1:A:588:LEU:CD1	2.86	0.48
1:A:690:ASP:C	1:A:691:VAL:HG23	2.38	0.48
1:E:80:GLU:O	1:E:81:MET:HE2	2.13	0.48
1:E:536:LEU:CD1	1:E:540:ILE:HD11	2.42	0.48
1:E:644:ASN:ND2	1:E:684:VAL:H	2.11	0.48
1:A:387:PRO:HG3	1:A:394:PHE:CE1	2.47	0.48
2:B:438:GLY:HA3	2:B:471:ILE:CD1	2.43	0.48
1:C:501:LEU:C	1:C:501:LEU:CD2	2.86	0.48
1:E:144:ARG:HG2	1:E:192:TYR:CD2	2.48	0.48
1:E:220:PHE:HA	1:E:224:GLN:OE1	2.12	0.48
1:E:237:LYS:HA	1:E:240:MET:CB	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:GLU:HB3	1:E:529:ILE:HD11	1.95	0.48
1:E:569:SER:O	1:E:720:ALA:HB1	2.14	0.48
1:A:521:TYR:CZ	1:A:529:ILE:HD12	2.48	0.48
1:C:120:ARG:NH1	1:C:479:LYS:HG3	2.29	0.48
1:C:647:ILE:HG13	1:C:685:ARG:NE	2.28	0.48
2:D:465:ILE:HG13	2:D:466:TRP:CD1	2.49	0.48
1:E:647:ILE:HG13	1:E:685:ARG:HE	1.78	0.48
1:E:685:ARG:NE	1:E:687:ASN:HD21	2.11	0.48
2:F:508:LEU:N	2:F:509:PRO:CD	2.77	0.48
1:A:130:ASP:OD1	1:A:159:LYS:HD2	2.14	0.48
1:A:167:LEU:HD12	1:A:167:LEU:N	2.28	0.48
1:C:172:GLU:HA	1:C:274:ASN:HD21	1.79	0.48
2:D:476:ALA:HA	2:D:582:LEU:HD23	1.95	0.48
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.95	0.48
1:E:325:ARG:HG2	1:E:325:ARG:HH11	1.79	0.48
1:E:677:PHE:CZ	1:E:679:GLU:HG3	2.49	0.48
2:B:438:GLY:HA3	2:B:471:ILE:HD13	1.96	0.48
2:B:450:ILE:HG23	2:B:455:VAL:HG23	1.96	0.48
1:C:571:SER:HB2	1:C:589:LYS:CG	2.43	0.48
1:E:412:ARG:HG2	1:E:412:ARG:NH1	2.29	0.48
1:E:528:HIS:O	1:E:529:ILE:HD13	2.14	0.48
1:A:91:GLN:HE22	1:A:343:PRO:HA	1.79	0.47
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.49	0.47
1:C:42:ARG:HG3	1:C:331:ALA:HB1	1.93	0.47
1:C:385:MET:SD	1:C:396:ALA:HA	2.54	0.47
1:C:647:ILE:HB	1:C:687:ASN:ND2	2.29	0.47
1:A:806:SER:HB2	1:A:813:SER:HB2	1.97	0.47
1:C:189:VAL:HG13	1:C:200:VAL:HG12	1.96	0.47
1:E:82:SER:O	1:E:86:VAL:HG23	2.14	0.47
1:E:181:THR:O	1:E:185:VAL:HG23	2.15	0.47
1:E:203:TYR:CD2	1:E:206:ARG:HD2	2.46	0.47
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.44	0.47
1:E:284:LEU:CD1	1:E:324:MET:HE1	2.43	0.47
1:E:606:ILE:HD12	1:E:619:MET:HG2	1.96	0.47
1:A:81:MET:O	1:A:96:ASN:HB3	2.14	0.47
1:A:225:PHE:CE2	1:A:277:ILE:HG23	2.49	0.47
1:A:408:GLY:O	1:A:409:GLN:C	2.57	0.47
1:A:647:ILE:CG1	1:A:685:ARG:HE	2.25	0.47
1:A:719:LEU:HD21	1:A:835:TRP:CE2	2.48	0.47
1:C:386:VAL:HG11	1:C:437:MET:CE	2.45	0.47
1:C:488:VAL:HG23	1:C:489:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:MET:HE3	1:E:436:LEU:HD13	1.97	0.47
1:E:129:VAL:HG12	1:E:130:ASP:N	2.28	0.47
2:F:427:ARG:O	2:F:428:GLN:C	2.55	0.47
2:F:470:TYR:CE2	2:F:555:ILE:HG12	2.50	0.47
1:A:569:SER:O	1:A:592:PRO:HD3	2.14	0.47
1:C:581:ASN:O	1:C:582:LYS:CB	2.62	0.47
1:C:655:TYR:O	1:C:656:LEU:C	2.57	0.47
1:C:760:ARG:O	1:C:761:PRO:C	2.58	0.47
2:D:488:ASP:OD1	2:D:489:ALA:N	2.47	0.47
1:E:10:ARG:NH1	1:E:449:PRO:HD2	2.20	0.47
1:E:436:LEU:HD23	1:E:454:ILE:CD1	2.44	0.47
2:B:560:LEU:O	2:B:560:LEU:HD22	2.14	0.47
2:D:570:ALA:HB3	2:D:591:GLU:OE1	2.15	0.47
1:E:172:GLU:HA	1:E:274:ASN:HD21	1.79	0.47
1:E:807:ASP:OD2	1:E:809:LEU:N	2.33	0.47
2:F:493:ILE:O	2:F:493:ILE:HG22	2.14	0.47
1:A:83:ASP:O	1:A:87:LYS:HG3	2.14	0.47
1:A:324:MET:HE2	1:A:324:MET:HA	1.95	0.47
2:B:542:ILE:HD12	2:B:543:THR:H	1.80	0.47
1:C:43:ALA:HB1	1:C:78:TYR:O	2.13	0.47
1:C:116:THR:HB	1:C:481:MET:CE	2.45	0.47
2:F:422:LEU:HD13	2:F:594:ILE:HD11	1.97	0.47
2:B:457:ALA:HB2	2:B:558:TRP:CE3	2.49	0.47
2:B:490:ARG:N	2:B:490:ARG:CD	2.77	0.47
1:C:186:ASN:HB3	1:C:201:GLN:HG2	1.97	0.47
1:C:231:LYS:CG	1:C:232:LYS:N	2.77	0.47
1:C:256:LYS:HE2	1:C:256:LYS:CA	2.24	0.47
1:C:268:PRO:O	1:C:269:LEU:HD23	2.15	0.47
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.96	0.47
1:C:411:VAL:HG12	1:C:412:ARG:N	2.29	0.47
1:C:565:GLU:CD	1:C:676:ILE:HB	2.40	0.47
2:D:429:LEU:HD21	2:D:565:VAL:HG11	1.96	0.47
1:E:155:VAL:HB	1:E:209:VAL:HG22	1.97	0.47
1:E:411:VAL:HG12	1:E:412:ARG:N	2.28	0.47
1:E:503:LYS:HB3	1:E:551:GLY:N	2.30	0.47
1:E:581:ASN:ND2	1:E:699:DDE:O	2.48	0.47
1:E:734:GLN:N	1:E:734:GLN:NE2	2.58	0.47
1:A:580:PRO:HD2	1:A:704:GLN:CD	2.40	0.47
1:C:484:SER:HB3	1:C:797:VAL:HG23	1.97	0.47
1:C:638:PRO:HB3	1:C:672:LYS:HG2	1.96	0.47
1:E:147:LEU:HD12	1:E:192:TYR:HB2	1.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:739:ALA:HB1	1:E:788:THR:HB	1.97	0.47
2:F:556:LEU:HD22	2:F:560:LEU:CD1	2.45	0.47
1:A:760:ARG:O	1:A:761:PRO:C	2.58	0.47
1:C:216:HIS:HE2	1:C:317:LYS:HZ1	1.57	0.47
1:C:729:PHE:CD2	1:C:774:VAL:HG22	2.50	0.47
2:D:465:ILE:HD12	2:D:535:LEU:HD12	1.97	0.47
1:E:773:PRO:HB2	1:E:776:GLU:HB2	1.97	0.47
1:A:348:ALA:O	1:A:352:ARG:HB2	2.15	0.47
2:B:546:GLU:HG3	2:B:553:GLU:OE1	2.15	0.47
2:B:552:LEU:N	2:B:552:LEU:CD1	2.70	0.47
1:C:223:ARG:HH11	1:C:223:ARG:HG2	1.80	0.47
1:C:809:LEU:O	1:C:811:PRO:HD3	2.14	0.47
2:D:523:ALA:O	2:D:524:ALA:C	2.57	0.47
1:E:284:LEU:HD13	1:E:324:MET:CE	2.45	0.47
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.50	0.47
2:F:427:ARG:CG	2:F:428:GLN:N	2.78	0.47
1:A:112:SER:CB	1:A:794:PRO:O	2.63	0.46
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.78	0.46
2:B:558:TRP:O	2:B:559:PRO:C	2.55	0.46
1:E:386:VAL:HG11	1:E:437:MET:CE	2.44	0.46
1:A:118:ALA:O	1:A:122:THR:HG23	2.14	0.46
1:A:607:ASN:HB3	1:A:610:ASP:CG	2.40	0.46
2:B:556:LEU:HD22	2:B:560:LEU:CD1	2.45	0.46
1:C:546:GLU:HB2	1:C:554:LEU:HD12	1.98	0.46
1:E:607:ASN:HA	1:E:608:PRO:HD3	1.87	0.46
1:A:16:VAL:HG21	1:A:450:ALA:O	2.14	0.46
1:A:495:VAL:HA	1:A:554:LEU:HD23	1.97	0.46
1:A:620:ALA:HA	1:A:625:TRP:O	2.15	0.46
1:C:140:GLU:HG3	1:C:188:ILE:HD11	1.93	0.46
1:C:588:LEU:C	1:C:588:LEU:CD1	2.87	0.46
1:E:307:LEU:HB2	1:E:312:LYS:CE	2.45	0.46
1:E:552:VAL:CG2	1:E:553:PRO:CD	2.80	0.46
1:E:829:LYS:HD2	1:E:829:LYS:N	2.30	0.46
1:A:103:ILE:HD12	1:A:122:THR:HG22	1.96	0.46
1:A:386:VAL:HG11	1:A:437:MET:CE	2.46	0.46
1:C:131:THR:HG21	1:C:163:ALA:HB2	1.96	0.46
1:C:147:LEU:HD11	1:C:189:VAL:HA	1.96	0.46
1:C:385:MET:H	1:C:465:LYS:HD2	1.79	0.46
1:C:539:GLU:HA	1:C:542:LEU:HD12	1.98	0.46
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.97	0.46
1:E:132:ILE:HD12	1:E:132:ILE:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:506:GLU:O	1:E:510:ARG:HG2	2.15	0.46
1:E:524:GLU:C	1:E:526:GLY:H	2.24	0.46
2:F:538:ARG:HD2	2:F:538:ARG:HA	1.49	0.46
1:A:7:ASP:HA	1:A:10:ARG:CD	2.44	0.46
1:E:39:LEU:HD11	1:E:334:LEU:CB	2.46	0.46
1:E:39:LEU:HD11	1:E:334:LEU:HD12	1.98	0.46
1:E:314:LEU:C	1:E:319:LEU:HB2	2.40	0.46
1:E:581:ASN:HB3	1:E:583:HIS:CD2	2.51	0.46
1:E:740:VAL:HG21	1:E:766:PHE:CD1	2.49	0.46
2:F:518:LEU:O	2:F:520:ALA:N	2.49	0.46
1:C:253:LYS:HA	1:C:253:LYS:CE	2.23	0.46
1:C:306:VAL:HG23	1:C:306:VAL:O	2.15	0.46
1:C:589:LYS:HE3	1:C:689:LEU:HD11	1.97	0.46
1:E:324:MET:HE2	1:E:324:MET:HA	1.98	0.46
1:E:595:GLU:OE2	1:E:682:ARG:NH2	2.41	0.46
1:E:710:ARG:HG3	1:E:710:ARG:HH11	1.81	0.46
1:E:784:LEU:CD2	1:E:794:PRO:HG3	2.38	0.46
1:E:829:LYS:HD2	1:E:829:LYS:H	1.81	0.46
1:A:365:ASN:O	1:A:369:ILE:HG12	2.16	0.46
1:C:235:VAL:CG1	1:C:236:ASP:N	2.79	0.46
1:C:374:PRO:O	1:C:404:THR:HG23	2.15	0.46
1:E:137:VAL:CG1	1:E:785:ARG:NH2	2.78	0.46
2:B:446:ALA:O	2:B:447:ALA:C	2.59	0.46
1:C:222:ILE:HG22	1:C:241:MET:HB2	1.98	0.46
1:C:552:VAL:CG2	1:C:553:PRO:CD	2.83	0.46
1:C:580:PRO:HD2	1:C:704:GLN:NE2	2.31	0.46
1:E:557:SER:O	1:E:558:PRO:O	2.33	0.46
1:E:647:ILE:HG13	1:E:685:ARG:NE	2.31	0.46
1:A:41:GLN:O	1:A:41:GLN:HG2	2.16	0.46
1:C:156:VAL:HG22	1:C:210:ALA:HB3	1.98	0.46
1:C:262:THR:OG1	1:C:263:ASP:N	2.49	0.46
1:E:345:PRO:HG2	1:E:451:GLY:O	2.16	0.46
1:E:493:VAL:CG1	1:E:494:GLU:N	2.79	0.46
1:A:436:LEU:HD23	1:A:454:ILE:CD1	2.46	0.46
1:A:757:GLU:HG3	1:A:768:VAL:HG22	1.97	0.46
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.45	0.46
1:C:218:TRP:C	1:C:330:ALA:HB2	2.41	0.46
1:C:331:ALA:O	1:C:335:LEU:HG	2.16	0.46
1:C:520:THR:HG22	1:C:530:VAL:HG22	1.97	0.46
1:E:545:LEU:HD12	1:E:549:HIS:CB	2.41	0.46
1:E:760:ARG:O	1:E:761:PRO:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.97	0.45
1:A:565:GLU:O	1:A:681:MET:HA	2.16	0.45
2:B:423:LEU:HD11	2:B:590:LYS:HD3	1.98	0.45
1:C:117:ALA:CA	1:C:481:MET:HE1	2.46	0.45
2:D:445:GLU:CD	2:D:494:ARG:HH22	2.23	0.45
2:D:542:ILE:HG12	2:D:543:THR:N	2.31	0.45
1:E:654:GLN:HG2	1:E:655:TYR:CG	2.52	0.45
1:E:705:ILE:N	1:E:705:ILE:HD12	2.31	0.45
2:F:436:PHE:HB2	2:F:502:TYR:CE2	2.50	0.45
1:A:710:ARG:HG3	1:A:710:ARG:NH1	2.32	0.45
1:A:730:LEU:HB2	1:A:799:ASP:HB2	1.98	0.45
2:B:490:ARG:HD2	2:B:490:ARG:H	1.82	0.45
1:C:45:ILE:HD11	1:C:78:TYR:HB3	1.95	0.45
1:E:202:VAL:HG23	1:E:202:VAL:O	2.16	0.45
1:E:348:ALA:HA	1:E:351:TYR:CZ	2.51	0.45
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.98	0.45
1:E:732:GLU:N	1:E:795:GLN:O	2.46	0.45
1:C:493:VAL:HG21	1:C:545:LEU:CD2	2.45	0.45
1:C:515:ASP:HB3	1:C:518:VAL:CG1	2.47	0.45
1:C:558:PRO:HA	1:C:559:PRO:HD3	1.79	0.45
1:C:685:ARG:HE	1:C:687:ASN:ND2	2.13	0.45
1:C:816:GLY:O	1:C:820:LEU:HB3	2.16	0.45
1:E:10:ARG:NH1	1:E:449:PRO:CD	2.59	0.45
1:E:117:ALA:HA	1:E:481:MET:SD	2.57	0.45
1:E:150:ARG:HH12	1:E:355:GLN:HB2	1.81	0.45
2:F:400:PHE:CD1	2:F:429:LEU:HD23	2.51	0.45
1:A:12:LEU:HG	1:A:99:LEU:HB2	1.96	0.45
1:A:296:ILE:N	1:A:297:PRO:HD2	2.31	0.45
2:B:417:TRP:CD1	2:B:568:PRO:HB2	2.51	0.45
1:C:277:ILE:HG22	1:C:278:LEU:N	2.31	0.45
1:C:311:GLU:OE2	1:C:322:VAL:CG1	2.64	0.45
1:E:137:VAL:HG13	1:E:785:ARG:NH2	2.31	0.45
1:E:143:LEU:O	1:E:147:LEU:HG	2.16	0.45
1:E:735:CYS:HA	1:E:736:PRO:HD3	1.81	0.45
2:F:558:TRP:O	2:F:559:PRO:C	2.57	0.45
1:C:250:PHE:HB3	1:C:275:MET:HE1	1.97	0.45
1:C:291:PHE:O	1:C:293:LYS:N	2.50	0.45
1:C:550:ALA:C	1:C:552:VAL:H	2.24	0.45
1:C:675:PRO:HD3	1:C:714:TYR:CD1	2.52	0.45
1:C:733:ILE:HG21	1:C:743:ILE:CD1	2.47	0.45
1:E:12:LEU:HG	1:E:99:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:LYS:NZ	1:E:106:PRO:O	2.49	0.45
1:E:485:VAL:HG22	1:E:485:VAL:O	2.17	0.45
1:A:126:LEU:HD11	1:A:156:VAL:HG23	1.99	0.45
1:A:454:ILE:CG1	1:A:455:GLY:H	2.27	0.45
1:A:647:ILE:HB	1:A:687:ASN:ND2	2.30	0.45
1:C:38:SER:CA	1:C:41:GLN:HG2	2.46	0.45
1:C:164:LEU:HD21	1:C:174:LEU:HD22	1.98	0.45
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.99	0.45
1:E:611:ASP:OD2	1:E:613:LYS:HB2	2.17	0.45
1:E:743:ILE:HD13	1:E:784:LEU:HD11	1.98	0.45
1:A:258:THR:HG21	1:A:260:LYS:HG2	1.97	0.45
1:A:338:ILE:O	1:A:342:LEU:HB2	2.17	0.45
1:A:561:VAL:HG21	1:A:775:ASN:CB	2.46	0.45
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.52	0.45
1:C:360:PRO:C	1:C:362:ASP:H	2.24	0.45
1:C:581:ASN:ND2	1:C:704:GLN:HG3	2.32	0.45
1:C:611:ASP:O	1:C:612:PHE:C	2.59	0.45
1:E:466:THR:HG22	1:E:467:GLY:N	2.32	0.45
1:E:507:GLY:CA	1:E:549:HIS:HB3	2.46	0.45
1:E:635:CYS:CB	1:E:664:VAL:HG13	2.46	0.45
1:E:823:ARG:NH2	1:E:833:PRO:HD3	2.31	0.45
2:B:474:ASP:OD1	2:B:475:PRO:HD2	2.16	0.45
2:B:484:ASP:OD2	2:B:494:ARG:N	2.50	0.45
1:C:45:ILE:HB	1:C:76:SER:HB2	1.99	0.45
1:C:82:SER:O	1:C:86:VAL:HG23	2.17	0.45
1:C:464:LEU:HD12	1:C:483:PHE:CZ	2.52	0.45
1:E:508:LEU:HD22	1:E:520:THR:CG2	2.47	0.45
1:E:712:ALA:O	1:E:715:ALA:HB3	2.17	0.45
1:A:380:LEU:C	1:A:380:LEU:HD23	2.42	0.45
1:C:111:PHE:HB3	1:C:114:GLU:HG2	1.99	0.45
1:C:523:SER:O	1:C:526:GLY:N	2.50	0.45
1:C:729:PHE:HB2	1:C:772:LEU:O	2.17	0.45
2:D:535:LEU:HB3	2:D:536:PRO:HA	1.99	0.45
2:D:561:ALA:O	2:D:564:THR:HG23	2.17	0.45
1:E:4:PHE:HD1	1:E:8:GLN:CD	2.24	0.45
1:E:149:GLU:O	1:E:150:ARG:HB2	2.16	0.45
2:F:450:ILE:O	2:F:454:GLY:N	2.50	0.45
1:A:7:ASP:O	1:A:10:ARG:CG	2.65	0.45
1:C:542:LEU:O	1:C:545:LEU:HB3	2.17	0.45
1:C:578:LYS:HE2	1:C:840:ASP:CG	2.40	0.45
1:C:693:LEU:HB3	1:C:700:ARG:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:471:ILE:HG13	2:D:554:THR:HB	1.97	0.45
2:D:541:ALA:HB2	2:D:556:LEU:HD23	1.99	0.45
1:E:306:VAL:HG23	1:E:306:VAL:O	2.17	0.45
1:E:520:THR:HA	1:E:529:ILE:O	2.17	0.45
2:F:443:PHE:CE2	2:F:445:GLU:HB2	2.52	0.45
2:F:498:LEU:HA	2:F:498:LEU:HD23	1.72	0.45
1:A:4:PHE:HD1	1:A:8:GLN:CD	2.25	0.44
1:A:43:ALA:HB1	1:A:78:TYR:O	2.17	0.44
1:A:371:ASN:O	1:A:372:CYS:C	2.59	0.44
1:A:690:ASP:O	1:A:691:VAL:CG2	2.65	0.44
1:C:552:VAL:CG2	1:C:553:PRO:HD3	2.39	0.44
1:C:567:VAL:HG23	1:C:592:PRO:HG3	1.99	0.44
1:E:72:SER:HA	1:E:439:GLY:O	2.18	0.44
1:A:7:ASP:HA	1:A:10:ARG:HD3	1.99	0.44
1:A:249:PHE:CD2	1:A:249:PHE:N	2.85	0.44
1:C:116:THR:HB	1:C:481:MET:HE3	1.99	0.44
1:C:129:VAL:HB	1:C:157:ILE:HD13	1.98	0.44
1:C:211:PHE:N	1:C:211:PHE:CD2	2.85	0.44
1:C:251:ASN:HA	1:C:252:PRO:HD3	1.64	0.44
1:C:490:GLN:HB2	1:C:529:ILE:CG2	2.47	0.44
1:C:507:GLY:O	1:C:511:LEU:HB2	2.17	0.44
1:C:735:CYS:SG	1:C:739:ALA:HB3	2.58	0.44
1:E:109:VAL:HG12	1:E:109:VAL:O	2.16	0.44
1:E:386:VAL:HA	1:E:387:PRO:HD3	1.79	0.44
1:C:218:TRP:CA	1:C:330:ALA:HB2	2.47	0.44
1:C:225:PHE:CE2	1:C:277:ILE:HG23	2.51	0.44
1:C:381:TYR:O	1:C:398:GLY:HA3	2.18	0.44
1:E:111:PHE:O	1:E:112:SER:C	2.59	0.44
1:E:158:ASN:HA	1:E:212:GLY:O	2.17	0.44
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.53	0.44
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.18	0.44
1:A:582:LYS:HE3	1:A:582:LYS:HB3	1.49	0.44
1:A:736:PRO:O	1:A:737:GLU:C	2.61	0.44
1:C:413:ILE:HD13	1:C:459:ILE:HG23	1.98	0.44
1:C:644:ASN:HD22	1:C:684:VAL:HB	1.82	0.44
1:E:4:PHE:HA	1:E:8:GLN:OE1	2.18	0.44
1:E:25:ILE:HG12	1:E:125:ALA:HB1	1.99	0.44
1:A:7:ASP:C	1:A:10:ARG:HG2	2.42	0.44
1:A:30:HIS:HA	1:A:159:LYS:NZ	2.32	0.44
1:A:32:LYS:HZ1	1:A:105:SER:HB2	1.79	0.44
1:A:581:ASN:HB3	1:A:583:HIS:ND1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ARG:HG3	1:C:331:ALA:HB2	1.90	0.44
1:C:109:VAL:CG1	1:C:793:PHE:CE1	3.01	0.44
1:C:223:ARG:HG2	1:C:223:ARG:NH1	2.33	0.44
1:E:500:ASP:HA	1:E:503:LYS:HD2	1.98	0.44
1:E:571:SER:HB2	1:E:589:LYS:CG	2.47	0.44
1:E:663:VAL:HG13	1:E:709:MET:SD	2.57	0.44
1:A:782:GLY:O	1:A:785:ARG:HB3	2.17	0.44
1:E:349:GLN:O	1:E:370:LYS:HA	2.17	0.44
1:E:360:PRO:C	1:E:362:ASP:H	2.25	0.44
1:E:644:ASN:HD22	1:E:684:VAL:H	1.66	0.44
2:F:518:LEU:HD22	2:F:518:LEU:N	2.32	0.44
1:A:112:SER:HB3	1:A:794:PRO:O	2.18	0.44
1:A:200:VAL:O	1:A:200:VAL:CG1	2.65	0.44
1:A:550:ALA:C	1:A:552:VAL:N	2.76	0.44
2:B:490:ARG:CD	2:B:490:ARG:H	2.31	0.44
1:C:251:ASN:H	1:C:251:ASN:ND2	2.14	0.44
1:C:296:ILE:N	1:C:297:PRO:HD2	2.33	0.44
1:C:500:ASP:HB3	1:C:552:VAL:HG11	2.00	0.44
1:E:503:LYS:HB3	1:E:551:GLY:H	1.83	0.44
1:A:357:TYR:CE2	1:A:359:GLY:HA3	2.53	0.44
1:A:589:LYS:HE3	1:A:689:LEU:CD1	2.45	0.44
2:B:447:ALA:HA	2:B:499:LEU:HD21	2.00	0.44
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.98	0.44
1:C:108:HIS:HD2	1:C:110:ASP:H	1.65	0.44
1:C:224:GLN:O	1:C:228:ARG:HG3	2.18	0.44
1:C:499:ASN:C	1:C:501:LEU:H	2.26	0.44
2:D:531:ILE:CD1	2:D:533:HIS:CE1	2.94	0.44
1:E:79:SER:O	1:E:98:PHE:N	2.50	0.44
1:E:338:ILE:HA	1:E:342:LEU:HG	1.99	0.44
1:E:613:LYS:O	1:E:616:ALA:HB3	2.18	0.44
1:E:700:ARG:O	1:E:705:ILE:HD13	2.17	0.44
1:A:258:THR:CG2	1:A:260:LYS:HG2	2.48	0.44
1:A:491:VAL:HG13	1:A:538:LEU:HD21	2.00	0.44
1:A:550:ALA:C	1:A:552:VAL:H	2.26	0.44
1:E:118:ALA:O	1:E:122:THR:HG23	2.18	0.44
1:E:274:ASN:O	1:E:279:ASP:HB2	2.17	0.44
1:E:588:LEU:C	1:E:588:LEU:CD1	2.90	0.44
1:E:619:MET:HE1	1:E:633:ILE:CD1	2.47	0.44
1:E:685:ARG:HE	1:E:687:ASN:ND2	2.15	0.44
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.57	0.44
1:A:39:LEU:HB3	1:A:77:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:HG23	1:A:489:VAL:CG2	2.48	0.43
1:A:538:LEU:O	1:A:539:GLU:C	2.61	0.43
2:B:479:TYR:CD2	2:B:582:LEU:HB2	2.53	0.43
2:B:516:LEU:O	2:B:545:PRO:HD2	2.18	0.43
1:C:317:LYS:HD2	1:C:317:LYS:HA	1.28	0.43
1:C:411:VAL:HG12	1:C:412:ARG:O	2.17	0.43
1:E:389:SER:O	1:E:391:LYS:N	2.51	0.43
1:E:694:HIS:NE2	1:E:699:DDE:HD2	2.33	0.43
2:F:479:TYR:CG	2:F:582:LEU:HB2	2.53	0.43
1:A:19:VAL:HA	1:A:99:LEU:O	2.18	0.43
1:A:522:MET:HE3	1:A:526:GLY:O	2.17	0.43
2:B:444:LEU:O	2:B:445:GLU:C	2.60	0.43
2:B:577:ASN:C	2:B:577:ASN:HD22	2.26	0.43
1:C:521:TYR:CD1	1:C:529:ILE:HD13	2.52	0.43
1:C:717:PHE:C	1:C:717:PHE:CD2	2.96	0.43
1:C:734:GLN:HE21	1:C:734:GLN:CA	2.29	0.43
1:E:68:ILE:HG21	1:E:395:TYR:OH	2.18	0.43
1:E:381:TYR:OH	1:E:481:MET:HG3	2.18	0.43
2:F:467:ARG:HG3	2:F:558:TRP:NE1	2.33	0.43
1:A:19:VAL:HG22	1:A:99:LEU:HB3	2.00	0.43
1:A:414:GLN:HB3	1:A:418:TYR:CD2	2.52	0.43
1:A:558:PRO:HA	1:A:559:PRO:HD3	1.92	0.43
1:C:16:VAL:HG12	1:C:346:VAL:HG23	2.00	0.43
1:C:557:SER:O	1:C:558:PRO:C	2.62	0.43
1:C:606:ILE:HD12	1:C:619:MET:CG	2.48	0.43
1:E:296:ILE:N	1:E:297:PRO:HD2	2.34	0.43
2:F:476:ALA:HA	2:F:582:LEU:HD23	2.01	0.43
1:A:654:GLN:HG2	1:A:655:TYR:CG	2.54	0.43
1:C:156:VAL:HG21	1:C:334:LEU:HD22	2.00	0.43
2:D:436:PHE:CE1	2:D:438:GLY:O	2.71	0.43
1:E:4:PHE:CE2	1:E:45:ILE:HD12	2.53	0.43
1:E:153:PRO:HD2	1:E:200:VAL:CG2	2.48	0.43
1:E:461:GLN:NE2	1:E:462:PHE:CE2	2.87	0.43
1:E:749:LYS:HG3	1:E:750:LYS:HD2	1.98	0.43
1:C:411:VAL:HG13	1:C:470:THR:O	2.19	0.43
2:D:437:VAL:HG11	2:D:511:PHE:CE2	2.54	0.43
2:F:443:PHE:CD2	2:F:445:GLU:HB2	2.53	0.43
1:A:549:HIS:CD2	1:A:549:HIS:H	2.35	0.43
1:A:733:ILE:O	1:A:767:THR:HA	2.19	0.43
2:B:489:ALA:HB3	2:B:490:ARG:HH11	1.82	0.43
1:C:262:THR:CA	1:C:269:LEU:HG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ILE:CG2	1:C:319:LEU:HG	2.47	0.43
1:C:387:PRO:HG3	1:C:394:PHE:CE1	2.54	0.43
1:C:411:VAL:CG1	1:C:412:ARG:N	2.81	0.43
1:C:659:ILE:HD13	1:C:693:LEU:HD21	2.00	0.43
2:D:470:TYR:CE2	2:D:555:ILE:HD11	2.54	0.43
1:A:569:SER:O	1:A:720:ALA:HB1	2.18	0.43
1:A:580:PRO:HB2	1:A:704:GLN:HE22	1.83	0.43
1:A:611:ASP:O	1:A:612:PHE:C	2.61	0.43
2:D:541:ALA:CB	2:D:556:LEU:HD23	2.49	0.43
1:E:229:TYR:CD1	1:E:232:LYS:HD2	2.54	0.43
1:E:350:ALA:O	1:E:370:LYS:HG2	2.18	0.43
1:E:490:GLN:HA	1:E:531:ALA:HA	2.01	0.43
1:E:782:GLY:O	1:E:786:GLN:NE2	2.52	0.43
1:A:228:ARG:C	1:A:230:ALA:N	2.77	0.43
1:A:504:LEU:HD22	1:A:554:LEU:CD2	2.49	0.43
1:A:522:MET:CE	1:A:526:GLY:O	2.66	0.43
1:A:565:GLU:CD	1:A:676:ILE:HB	2.44	0.43
1:A:626:ASP:O	1:A:627:VAL:C	2.59	0.43
1:A:824:LYS:HE3	1:A:830:GLU:OE2	2.19	0.43
1:C:494:GLU:OE1	1:C:494:GLU:CA	2.66	0.43
1:A:240:MET:O	1:A:244:LEU:HG	2.18	0.43
1:A:704:GLN:O	1:A:707:PRO:HD2	2.19	0.43
1:C:186:ASN:CB	1:C:201:GLN:HG2	2.49	0.43
1:C:276:PHE:C	1:C:277:ILE:HD12	2.44	0.43
1:C:459:ILE:O	1:C:462:PHE:N	2.48	0.43
1:C:497:ASN:HD22	1:C:497:ASN:H	1.67	0.43
1:E:171:LYS:HZ3	1:E:283:ARG:HH21	1.67	0.43
1:E:209:VAL:HG12	1:E:211:PHE:CE1	2.53	0.43
1:A:411:VAL:HG13	1:A:470:THR:O	2.19	0.43
1:A:591:GLU:OE2	1:A:685:ARG:NH1	2.52	0.43
2:B:499:LEU:HB3	2:B:566:VAL:CG1	2.49	0.43
2:B:583:ASP:HA	2:B:584:PRO:HD2	1.86	0.43
1:C:253:LYS:HG3	1:C:253:LYS:O	2.19	0.43
1:C:587:TYR:CD2	1:C:690:ASP:HB3	2.53	0.43
1:C:646:VAL:HG13	1:C:688:ILE:HD13	2.01	0.43
1:C:749:LYS:O	1:C:750:LYS:HD2	2.19	0.43
1:E:4:PHE:CD2	1:E:45:ILE:HD12	2.54	0.43
2:B:503:VAL:HB	2:B:504:PRO:CD	2.49	0.42
2:B:520:ALA:HB1	2:B:521:PRO:CD	2.48	0.42
1:C:694:HIS:HD2	1:C:696:ASP:N	2.00	0.42
1:E:737:GLU:HG3	1:E:766:PHE:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HG12	1:A:345:PRO:HG2	1.94	0.42
1:A:597:VAL:O	1:A:601:ILE:HG13	2.20	0.42
1:A:711:ARG:HH11	2:B:577:ASN:HD21	1.67	0.42
2:B:518:LEU:H	2:B:518:LEU:CD2	2.33	0.42
1:C:285:PHE:CE2	1:C:324:MET:SD	3.09	0.42
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.85	0.42
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.34	0.42
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.54	0.42
1:A:729:PHE:CD2	1:A:774:VAL:HG22	2.54	0.42
2:B:458:ARG:O	2:B:459:SER:HB2	2.18	0.42
1:C:158:ASN:HD22	1:C:159:LYS:HG2	1.78	0.42
1:C:236:ASP:OD1	1:C:238:ALA:HB3	2.19	0.42
1:E:681:MET:HE2	1:E:717:PHE:CD1	2.54	0.42
1:E:800:HIS:CD2	1:E:800:HIS:N	2.87	0.42
1:E:814:LYS:O	1:E:817:GLU:HB3	2.20	0.42
1:A:488:VAL:HG23	1:A:489:VAL:HG23	2.01	0.42
1:A:591:GLU:HG2	1:A:685:ARG:CG	2.46	0.42
1:A:655:TYR:O	1:A:656:LEU:C	2.62	0.42
1:C:494:GLU:HG2	1:C:528:HIS:HE1	1.85	0.42
2:D:443:PHE:O	2:D:444:LEU:C	2.63	0.42
2:F:401:LEU:O	2:F:421:ARG:NE	2.48	0.42
1:A:626:ASP:O	1:A:628:THR:N	2.53	0.42
2:B:523:ALA:O	2:B:524:ALA:C	2.62	0.42
1:C:314:LEU:HG	1:C:318:ALA:C	2.45	0.42
1:C:410:LYS:HE2	1:C:430:ALA:HB2	2.02	0.42
1:C:522:MET:SD	1:C:528:HIS:HA	2.59	0.42
1:C:650:THR:CG2	1:C:688:ILE:HG22	2.50	0.42
1:C:690:ASP:OD1	1:C:691:VAL:N	2.47	0.42
1:C:840:ASP:CG	1:C:842:LEU:HD13	2.44	0.42
1:E:564:ARG:HD3	1:E:801:TRP:CH2	2.55	0.42
1:E:698:ILE:N	1:E:698:ILE:HD13	2.35	0.42
2:F:474:ASP:O	2:F:475:PRO:C	2.62	0.42
1:A:644:ASN:HD22	1:A:684:VAL:H	1.68	0.42
2:B:410:SER:OG	2:B:412:ARG:HB3	2.19	0.42
1:C:4:PHE:HD2	1:C:45:ILE:HG23	1.84	0.42
1:C:216:HIS:NE2	1:C:317:LYS:NZ	2.62	0.42
1:C:525:SER:OG	1:C:527:GLU:HG3	2.20	0.42
1:C:534:GLY:O	1:C:535:GLU:C	2.62	0.42
2:D:498:LEU:HD23	2:D:498:LEU:HA	1.69	0.42
1:E:89:ILE:HG22	1:E:91:GLN:HB3	2.01	0.42
1:E:108:HIS:O	1:E:111:PHE:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:VAL:HB	1:E:209:VAL:CG2	2.49	0.42
1:E:749:LYS:C	1:E:750:LYS:HD2	2.45	0.42
1:A:556:ILE:HG22	1:A:557:SER:O	2.19	0.42
2:B:507:SER:C	2:B:509:PRO:HD2	2.43	0.42
1:C:155:VAL:O	1:C:337:MET:HE1	2.20	0.42
1:C:228:ARG:C	1:C:230:ALA:N	2.77	0.42
2:D:582:LEU:HD12	2:D:583:ASP:N	2.35	0.42
1:E:25:ILE:HD12	1:E:142:VAL:CG1	2.50	0.42
1:E:25:ILE:HD12	1:E:142:VAL:HG12	2.02	0.42
1:E:132:ILE:N	1:E:132:ILE:CD1	2.82	0.42
1:E:626:ASP:C	1:E:628:THR:N	2.77	0.42
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.54	0.42
2:F:531:ILE:HG22	2:F:533:HIS:H	1.85	0.42
1:A:46:ILE:HD12	1:A:46:ILE:HA	1.91	0.42
1:A:144:ARG:NH2	1:A:791:GLN:O	2.53	0.42
1:A:607:ASN:HA	1:A:608:PRO:HD3	1.82	0.42
2:B:484:ASP:OD2	2:B:494:ARG:CG	2.68	0.42
1:C:501:LEU:HD23	1:C:501:LEU:O	2.17	0.42
1:C:569:SER:O	1:C:592:PRO:HD3	2.20	0.42
2:D:507:SER:C	2:D:509:PRO:CD	2.93	0.42
1:E:121:VAL:HG11	1:E:383:SER:HB3	2.01	0.42
1:E:341:HIS:O	1:E:342:LEU:C	2.62	0.42
1:E:380:LEU:C	1:E:380:LEU:HD23	2.45	0.42
1:E:418:TYR:HD1	1:E:424:ASP:O	2.02	0.42
1:E:525:SER:O	2:F:412:ARG:CZ	2.67	0.42
1:A:590:ALA:HA	1:A:685:ARG:O	2.20	0.42
2:B:443:PHE:CD2	2:B:445:GLU:HB2	2.55	0.42
1:C:487:PRO:HB3	1:C:531:ALA:HB1	2.02	0.42
1:C:648:ASP:O	1:C:648:ASP:CG	2.62	0.42
1:E:78:TYR:CE1	1:E:97:SER:HB3	2.48	0.42
1:E:89:ILE:O	1:E:91:GLN:N	2.53	0.42
1:E:694:HIS:CE1	1:E:699:DDE:CD2	3.03	0.42
1:E:740:VAL:HG21	1:E:766:PHE:HD1	1.85	0.42
2:F:470:TYR:CD2	2:F:555:ILE:HG12	2.55	0.42
1:C:46:ILE:HD12	1:C:46:ILE:HA	1.92	0.42
1:C:237:LYS:O	1:C:241:MET:HG2	2.20	0.42
2:D:518:LEU:H	2:D:518:LEU:CD2	2.33	0.42
1:E:536:LEU:O	1:E:539:GLU:HB3	2.20	0.42
1:A:10:ARG:HG3	1:A:11:SER:N	2.35	0.41
1:A:380:LEU:HD23	1:A:381:TYR:N	2.35	0.41
1:A:600:ALA:HB1	1:A:606:ILE:HG12	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:LEU:O	1:C:427:PHE:CD1	2.73	0.41
1:C:511:LEU:HD22	1:C:545:LEU:HD13	2.02	0.41
1:C:543:GLN:O	1:C:547:HIS:N	2.46	0.41
1:C:739:ALA:HB2	1:C:791:GLN:OE1	2.20	0.41
2:D:518:LEU:HD11	2:D:542:ILE:HD13	2.02	0.41
2:D:570:ALA:O	2:D:572:PRO:HD3	2.20	0.41
1:E:515:ASP:HA	1:E:516:PRO:HD3	1.80	0.41
1:E:600:ALA:HB1	1:E:606:ILE:HG12	2.01	0.41
2:F:457:ALA:HB2	2:F:558:TRP:CD2	2.55	0.41
1:A:258:THR:CG2	1:A:259:ASN:N	2.79	0.41
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.89	0.41
1:C:19:VAL:HG12	1:C:20:ARG:N	2.35	0.41
1:C:73:THR:O	1:C:73:THR:HG22	2.21	0.41
1:C:161:ASP:CG	1:C:162:ARG:N	2.78	0.41
1:C:646:VAL:HG13	1:C:688:ILE:CD1	2.50	0.41
1:E:123:ASP:HB3	1:E:343:PRO:HG2	2.00	0.41
1:E:305:ILE:HG21	1:E:323:VAL:HG13	2.02	0.41
1:E:406:LYS:O	1:E:409:GLN:HB3	2.19	0.41
1:E:584:ASN:HD22	1:E:693:LEU:HA	1.84	0.41
1:E:655:TYR:O	1:E:656:LEU:C	2.62	0.41
1:E:804:LEU:N	1:E:804:LEU:HD23	2.35	0.41
1:A:395:TYR:CE1	1:A:457:VAL:HG13	2.55	0.41
1:A:556:ILE:HD12	1:A:556:ILE:N	2.35	0.41
2:B:535:LEU:HB3	2:B:536:PRO:HA	2.02	0.41
1:C:38:SER:HA	1:C:41:GLN:CG	2.49	0.41
1:C:192:TYR:HA	1:C:763:THR:HG22	2.02	0.41
1:C:530:VAL:O	1:C:538:LEU:HD11	2.21	0.41
1:C:609:ARG:NH1	1:C:609:ARG:HG3	2.35	0.41
1:E:144:ARG:HG2	1:E:192:TYR:CG	2.55	0.41
1:E:164:LEU:HD12	1:E:285:PHE:CE1	2.56	0.41
1:E:314:LEU:O	1:E:319:LEU:HB2	2.20	0.41
1:A:221:THR:OG1	1:A:224:GLN:HG3	2.20	0.41
1:A:503:LYS:HB2	1:A:552:VAL:HG21	2.01	0.41
2:B:447:ALA:O	2:B:448:GLN:C	2.63	0.41
2:B:518:LEU:HD22	2:B:518:LEU:N	2.34	0.41
1:C:192:TYR:HE1	1:C:765:LEU:HB2	1.86	0.41
1:C:274:ASN:HA	1:C:278:LEU:HB2	2.02	0.41
1:C:485:VAL:O	1:C:485:VAL:HG22	2.19	0.41
1:C:740:VAL:HG21	1:C:766:PHE:HB2	2.01	0.41
1:E:46:ILE:HG22	1:E:47:SER:N	2.27	0.41
1:E:239:LYS:NZ	1:E:243:ARG:NH2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:577:ASN:O	2:F:578:VAL:C	2.61	0.41
1:A:103:ILE:HD13	1:A:121:VAL:HG23	2.01	0.41
1:A:406:LYS:HB3	1:A:447:ASP:HB2	2.03	0.41
2:B:484:ASP:OD2	2:B:494:ARG:CD	2.69	0.41
1:C:418:TYR:HB3	1:C:477:ASN:HD21	1.85	0.41
1:C:501:LEU:N	1:C:502:PRO:CD	2.83	0.41
1:C:600:ALA:HB1	1:C:606:ILE:HG12	2.00	0.41
1:C:758:GLU:O	1:C:759:GLN:HB3	2.19	0.41
2:D:530:LEU:HD23	2:D:604:PRO:HD3	2.02	0.41
1:E:734:GLN:HE21	1:E:734:GLN:H	1.65	0.41
1:C:124:GLY:HA3	1:C:342:LEU:HD22	2.01	0.41
1:C:490:GLN:C	1:C:491:VAL:HG13	2.46	0.41
2:D:451:VAL:O	2:D:451:VAL:CG1	2.68	0.41
2:D:518:LEU:HD22	2:D:518:LEU:N	2.35	0.41
1:E:807:ASP:HA	1:E:808:PRO:HD2	1.95	0.41
2:F:423:LEU:HD11	2:F:590:LYS:HD3	2.03	0.41
2:F:571:ILE:HD11	2:F:587:ILE:HD12	2.02	0.41
1:A:606:ILE:HD12	1:A:619:MET:HG3	2.01	0.41
1:A:654:GLN:HG2	1:A:655:TYR:CE2	2.54	0.41
1:C:167:LEU:CD1	1:C:167:LEU:N	2.84	0.41
1:C:397:PHE:HD1	1:C:437:MET:HG3	1.86	0.41
1:C:804:LEU:HD23	1:C:804:LEU:N	2.35	0.41
1:E:126:LEU:HD11	1:E:156:VAL:HG23	2.00	0.41
1:A:27:HIS:CD2	1:A:29:ASP:HB2	2.56	0.41
1:A:124:GLY:HA3	1:A:342:LEU:HD22	2.02	0.41
1:A:512:SER:HA	1:A:518:VAL:CG1	2.51	0.41
2:B:450:ILE:HG23	2:B:455:VAL:CG2	2.51	0.41
1:E:10:ARG:HA	1:E:10:ARG:HD2	1.91	0.41
1:A:71:LYS:O	1:A:386:VAL:HG21	2.21	0.41
1:A:254:THR:O	1:A:255:LYS:HB2	2.21	0.41
1:A:363:ASP:O	1:A:367:ILE:HG13	2.21	0.41
1:A:571:SER:O	1:A:572:SER:C	2.64	0.41
2:B:467:ARG:HG3	2:B:558:TRP:HD1	1.84	0.41
1:C:80:GLU:C	1:C:81:MET:HG2	2.44	0.41
1:C:152:LYS:HD2	1:C:200:VAL:HG22	2.03	0.41
1:C:169:VAL:O	1:C:169:VAL:HG13	2.21	0.41
1:C:338:ILE:O	1:C:342:LEU:HB2	2.21	0.41
1:C:597:VAL:O	1:C:601:ILE:HG13	2.20	0.41
2:D:446:ALA:O	2:D:447:ALA:C	2.64	0.41
2:D:495:ASN:OD1	2:D:495:ASN:N	2.53	0.41
1:E:186:ASN:HA	1:E:189:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:THR:HG21	1:E:336:GLU:OE1	2.21	0.41
1:E:303:LEU:O	1:E:304:GLU:CB	2.69	0.41
1:E:397:PHE:HD1	1:E:437:MET:HG3	1.85	0.41
1:E:594:ASP:HB2	1:E:597:VAL:HG23	2.03	0.41
1:E:806:SER:HB2	1:E:813:SER:HB2	2.02	0.41
2:F:422:LEU:O	2:F:423:LEU:C	2.62	0.41
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.56	0.41
1:A:784:LEU:CD2	1:A:794:PRO:HG3	2.50	0.41
1:C:291:PHE:CE1	1:C:315:GLU:HB2	2.52	0.41
1:C:316:GLY:O	1:C:319:LEU:N	2.54	0.41
1:C:521:TYR:O	1:C:529:ILE:HD12	2.21	0.41
1:C:536:LEU:O	1:C:537:HIS:C	2.64	0.41
2:D:448:GLN:HE21	2:D:448:GLN:HB2	1.71	0.41
1:E:5:THR:OG1	1:E:8:GLN:HG3	2.21	0.41
1:E:39:LEU:HD11	1:E:334:LEU:HB2	2.03	0.41
1:E:70:ILE:HA	1:E:388:THR:HA	2.03	0.41
1:E:156:VAL:CG2	1:E:337:MET:HE1	2.51	0.41
1:E:262:THR:HG21	1:E:266:GLY:HA2	2.02	0.41
2:F:464:ALA:O	2:F:467:ARG:HB3	2.21	0.41
1:A:82:SER:C	1:A:84:GLU:N	2.79	0.40
2:B:457:ALA:C	2:B:458:ARG:HG3	2.46	0.40
1:C:379:MET:SD	1:C:470:THR:HG22	2.61	0.40
1:C:384:LYS:HB2	1:C:465:LYS:HZ2	1.85	0.40
1:C:495:VAL:CG1	1:C:554:LEU:HD23	2.50	0.40
1:C:626:ASP:O	1:C:627:VAL:C	2.63	0.40
1:C:799:ASP:OD1	1:C:800:HIS:HD2	2.04	0.40
1:E:731:VAL:HG13	1:E:731:VAL:O	2.20	0.40
1:E:797:VAL:HG22	1:E:798:PHE:N	2.35	0.40
2:F:400:PHE:O	2:F:425:ALA:HB1	2.20	0.40
1:A:91:GLN:O	1:A:93:THR:HG23	2.21	0.40
1:A:576:LEU:HD13	1:A:587:TYR:CD1	2.56	0.40
1:A:700:ARG:HE	1:A:700:ARG:HB2	1.49	0.40
1:E:189:VAL:O	1:E:193:ALA:CB	2.69	0.40
1:E:205:ALA:HB2	1:E:245:TRP:HB3	2.02	0.40
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.86	0.40
1:E:391:LYS:CG	1:E:392:GLY:H	2.34	0.40
1:E:500:ASP:O	1:E:503:LYS:N	2.50	0.40
1:E:810:ASP:OD1	1:E:810:ASP:C	2.64	0.40
1:E:823:ARG:NH1	1:E:823:ARG:HG2	2.36	0.40
2:F:429:LEU:O	2:F:434:TYR:HB2	2.22	0.40
1:A:26:ALA:CB	1:A:128:VAL:HB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:O	1:A:112:SER:C	2.64	0.40
1:A:404:THR:HB	1:A:447:ASP:OD2	2.21	0.40
1:A:694:HIS:HD2	1:A:696:ASP:N	1.99	0.40
1:C:237:LYS:HA	1:C:240:MET:HB3	2.04	0.40
1:C:506:GLU:C	1:C:508:LEU:N	2.77	0.40
2:D:557:GLY:O	2:D:558:TRP:C	2.64	0.40
1:E:74:ALA:O	1:E:439:GLY:CA	2.67	0.40
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.57	0.40
1:E:167:LEU:H	1:E:167:LEU:CD1	2.34	0.40
1:E:388:THR:HG21	1:E:395:TYR:CD1	2.56	0.40
2:F:451:VAL:O	2:F:451:VAL:HG12	2.17	0.40
1:A:40:VAL:C	1:A:42:ARG:H	2.30	0.40
1:A:713:THR:O	1:A:714:TYR:C	2.62	0.40
2:B:507:SER:C	2:B:509:PRO:CD	2.94	0.40
1:C:111:PHE:O	1:C:112:SER:C	2.63	0.40
1:C:411:VAL:HG11	1:C:469:LEU:HB3	2.04	0.40
1:C:454:ILE:CG1	1:C:455:GLY:N	2.85	0.40
1:C:591:GLU:OE2	1:C:685:ARG:NH1	2.55	0.40
1:E:68:ILE:HG23	1:E:390:ASP:CB	2.50	0.40
1:E:169:VAL:CG2	1:E:173:ASP:HB2	2.51	0.40
1:A:512:SER:HA	1:A:518:VAL:HG13	2.04	0.40
1:A:644:ASN:ND2	1:A:684:VAL:HB	2.31	0.40
1:C:146:ALA:O	1:C:151:ILE:HG12	2.22	0.40
1:C:319:LEU:O	1:C:323:VAL:HG23	2.20	0.40
1:C:591:GLU:HA	1:C:592:PRO:HD3	1.84	0.40
1:C:736:PRO:O	1:C:739:ALA:N	2.52	0.40
2:D:436:PHE:HB2	2:D:502:TYR:CE2	2.56	0.40
2:D:479:TYR:CD2	2:D:582:LEU:HB2	2.56	0.40
1:E:500:ASP:CG	1:E:552:VAL:HG21	2.45	0.40
2:F:535:LEU:HB3	2:F:536:PRO:HA	2.04	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	818/842 (97%)	729 (89%)	75 (9%)	14 (2%)	7	27
1	C	818/842 (97%)	716 (88%)	80 (10%)	22 (3%)	4	18
1	E	818/842 (97%)	712 (87%)	90 (11%)	16 (2%)	6	23
2	B	205/207 (99%)	181 (88%)	22 (11%)	2 (1%)	12	39
2	D	205/207 (99%)	182 (89%)	17 (8%)	6 (3%)	3	17
2	F	205/207 (99%)	179 (87%)	21 (10%)	5 (2%)	4	20
All	All	3069/3147 (98%)	2699 (88%)	305 (10%)	65 (2%)	5	22

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	761	PRO
2	B	518	LEU
2	B	519	ALA
1	C	235	VAL
1	C	264	ALA
1	C	761	PRO
2	D	518	LEU
2	D	519	ALA
1	E	112	SER
1	E	558	PRO
1	E	761	PRO
2	F	519	ALA
1	A	309	GLY
1	A	390	ASP
1	A	498	ALA
1	C	112	SER
1	C	309	GLY
1	C	460	ASP
1	C	549	HIS
1	C	551	GLY
1	C	737	GLU
2	D	491	GLY
1	E	304	GLU
1	E	390	ASP
1	E	479	LYS
2	F	454	GLY

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Mol	Chain	Res	Type
1	A	111	PHE
1	A	237	LYS
1	A	479	LYS
1	C	266	GLY
1	C	479	LYS
1	E	90	LYS
1	E	233	PHE
2	F	577	ASN
1	A	460	ASP
1	A	677	PHE
1	C	265	GLU
1	C	314	LEU
1	C	558	PRO
1	C	743	ILE
1	C	785	ARG
1	E	372	CYS
1	E	621	ASP
1	A	446	ASP
1	C	120	ARG
1	C	329	PRO
1	C	446	ASP
1	C	525	SER
2	D	604	PRO
1	E	446	ASP
1	E	737	GLU
1	E	743	ILE
2	F	404	GLY
1	A	621	ASP
1	E	428	ILE
2	D	404	GLY
2	D	405	GLY
1	E	338	ILE
2	F	450	ILE
1	C	491	VAL
1	A	604	GLY
1	A	329	PRO
1	E	556	ILE
1	C	604	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	699/714 (98%)	654 (94%)	45 (6%)	16	42
1	C	699/714 (98%)	635 (91%)	64 (9%)	8	29
1	E	699/714 (98%)	656 (94%)	43 (6%)	16	43
2	B	161/162 (99%)	145 (90%)	16 (10%)	7	27
2	D	161/162 (99%)	143 (89%)	18 (11%)	6	22
2	F	161/162 (99%)	143 (89%)	18 (11%)	6	22
All	All	2580/2628 (98%)	2376 (92%)	204 (8%)	11	35

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	15	LYS
1	A	36	THR
1	A	46	ILE
1	A	68	ILE
1	A	81	MET
1	A	83	ASP
1	A	113	SER
1	A	152	LYS
1	A	154	VAL
1	A	162	ARG
1	A	200	VAL
1	A	236	ASP
1	A	261	ASP
1	A	262	THR
1	A	275	MET
1	A	300	LEU
1	A	308	LYS
1	A	347	THR
1	A	352	ARG
1	A	362	ASP
1	A	432	GLN

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Mol	Chain	Res	Type
1	A	460	ASP
1	A	489	VAL
1	A	536	LEU
1	A	582	LYS
1	A	597	VAL
1	A	599	LEU
1	A	609	ARG
1	A	625	TRP
1	A	677	PHE
1	A	698	ILE
1	A	710	ARG
1	A	718	LEU
1	A	723	LYS
1	A	724	ILE
1	A	730	LEU
1	A	734	GLN
1	A	738	GLN
1	A	761	PRO
1	A	767	THR
1	A	775	ASN
1	A	804	LEU
1	A	836	GLN
1	A	842	LEU
2	B	420	GLU
2	B	422	LEU
2	B	456	ARG
2	B	467	ARG
2	B	488	ASP
2	B	494	ARG
2	B	495	ASN
2	B	499	LEU
2	B	506	SER
2	B	540	ASP
2	B	547	GLU
2	B	551	ARG
2	B	552	LEU
2	B	559	PRO
2	B	560	LEU
2	B	602	SER
1	C	14	ASP
1	C	36	THR
1	C	46	ILE

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Mol	Chain	Res	Type
1	C	68	ILE
1	C	81	MET
1	C	83	ASP
1	C	94	ASP
1	C	105	SER
1	C	113	SER
1	C	154	VAL
1	C	159	LYS
1	C	164	LEU
1	C	167	LEU
1	C	172	GLU
1	C	183	GLU
1	C	195	GLU
1	C	200	VAL
1	C	231	LYS
1	C	235	VAL
1	C	242	ASP
1	C	253	LYS
1	C	269	LEU
1	C	299	LEU
1	C	300	LEU
1	C	301	GLU
1	C	317	LYS
1	C	320	LEU
1	C	324	MET
1	C	347	THR
1	C	362	ASP
1	C	432	GLN
1	C	460	ASP
1	C	461	GLN
1	C	489	VAL
1	C	494	GLU
1	C	495	VAL
1	C	497	ASN
1	C	499	ASN
1	C	500	ASP
1	C	506	GLU
1	C	524	GLU
1	C	528	HIS
1	C	529	ILE
1	C	552	VAL
1	C	556	ILE

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Mol	Chain	Res	Type
1	C	597	VAL
1	C	599	LEU
1	C	609	ARG
1	C	625	TRP
1	C	677	PHE
1	C	718	LEU
1	C	723	LYS
1	C	730	LEU
1	C	734	GLN
1	C	738	GLN
1	C	757	GLU
1	C	761	PRO
1	C	767	THR
1	C	775	ASN
1	C	804	LEU
1	C	820	LEU
1	C	828	MET
1	C	836	GLN
1	C	837	GLU
2	D	403	ASP
2	D	410	SER
2	D	411	THR
2	D	422	LEU
2	D	427	ARG
2	D	467	ARG
2	D	483	GLN
2	D	488	ASP
2	D	494	ARG
2	D	499	LEU
2	D	538	ARG
2	D	540	ASP
2	D	547	GLU
2	D	551	ARG
2	D	552	LEU
2	D	560	LEU
2	D	602	SER
2	D	604	PRO
1	E	23	SER
1	E	36	THR
1	E	46	ILE
1	E	87	LYS
1	E	94	ASP

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Mol	Chain	Res	Type
1	E	161	ASP
1	E	166	GLU
1	E	183	GLU
1	E	186	ASN
1	E	211	PHE
1	E	216	HIS
1	E	262	THR
1	E	263	ASP
1	E	275	MET
1	E	300	LEU
1	E	313	ASP
1	E	347	THR
1	E	362	ASP
1	E	440	ARG
1	E	460	ASP
1	E	489	VAL
1	E	527	GLU
1	E	552	VAL
1	E	558	PRO
1	E	576	LEU
1	E	597	VAL
1	E	599	LEU
1	E	625	TRP
1	E	677	PHE
1	E	688	ILE
1	E	698	ILE
1	E	710	ARG
1	E	718	LEU
1	E	724	ILE
1	E	730	LEU
1	E	734	GLN
1	E	738	GLN
1	E	749	LYS
1	E	761	PRO
1	E	767	THR
1	E	786	GLN
1	E	836	GLN
1	E	837	GLU
2	F	411	THR
2	F	422	LEU
2	F	467	ARG
2	F	494	ARG

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Mol	Chain	Res	Type
2	F	498	LEU
2	F	499	LEU
2	F	513	ARG
2	F	522	GLU
2	F	531	ILE
2	F	538	ARG
2	F	540	ASP
2	F	547	GLU
2	F	552	LEU
2	F	559	PRO
2	F	560	LEU
2	F	599	ASP
2	F	602	SER
2	F	604	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	30	HIS
1	A	91	GLN
1	A	101	ASN
1	A	138	GLN
1	A	176	GLN
1	A	201	GLN
1	A	274	ASN
1	A	414	GLN
1	A	528	HIS
1	A	537	HIS
1	A	547	HIS
1	A	549	HIS
1	A	581	ASN
1	A	584	ASN
1	A	644	ASN
1	A	654	GLN
1	A	687	ASN
1	A	694	HIS
1	A	734	GLN
1	A	738	GLN
1	A	748	ASN
1	A	753	GLN
1	A	800	HIS

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Mol	Chain	Res	Type
1	A	836	GLN
2	B	424	GLN
2	B	448	GLN
2	B	495	ASN
2	B	577	ASN
2	B	592	GLN
2	B	603	GLN
1	C	21	ASN
1	C	27	HIS
1	C	91	GLN
1	C	101	ASN
1	C	138	GLN
1	C	201	GLN
1	C	259	ASN
1	C	371	ASN
1	C	414	GLN
1	C	452	ASN
1	C	477	ASN
1	C	497	ASN
1	C	528	HIS
1	C	537	HIS
1	C	547	HIS
1	C	549	HIS
1	C	583	HIS
1	C	584	ASN
1	C	644	ASN
1	C	687	ASN
1	C	694	HIS
1	C	734	GLN
1	C	738	GLN
1	C	748	ASN
1	C	753	GLN
1	C	800	HIS
1	C	836	GLN
2	D	424	GLN
2	D	428	GLN
2	D	448	GLN
2	D	460	GLN
2	D	577	ASN
2	D	592	GLN
1	E	27	HIS
1	E	91	GLN

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Mol	Chain	Res	Type
1	E	101	ASN
1	E	138	GLN
1	E	201	GLN
1	E	259	ASN
1	E	371	ASN
1	E	414	GLN
1	E	528	HIS
1	E	537	HIS
1	E	547	HIS
1	E	549	HIS
1	E	581	ASN
1	E	583	HIS
1	E	584	ASN
1	E	644	ASN
1	E	654	GLN
1	E	687	ASN
1	E	694	HIS
1	E	734	GLN
1	E	753	GLN
1	E	800	HIS
1	E	836	GLN
2	F	428	GLN
2	F	448	GLN
2	F	460	GLN
2	F	577	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	DDE	E	699	1	9,10,21	0.44	0	8,12,30	0.98	0
1	DDE	C	699	1	9,10,21	0.40	0	8,12,30	0.99	0
1	DDE	A	699	1	9,10,21	0.45	0	8,12,30	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDE	E	699	1	-	0/5/6/23	0/1/1/1
1	DDE	C	699	1	-	0/5/6/23	0/1/1/1
1	DDE	A	699	1	-	0/5/6/23	0/1/1/1

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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	699	DDE	4	0
1	C	699	DDE	1	0
1	A	699	DDE	1	0

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 ⓘ

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	822/842 (97%)	0.26	12 (1%) 72 50	8, 57, 85, 104	0
1	C	822/842 (97%)	0.61	59 (7%) 21 11	10, 69, 123, 135	0
1	E	822/842 (97%)	1.32	200 (24%) 2 1	6, 105, 128, 146	0
2	B	207/207 (100%)	-0.21	6 (2%) 53 31	5, 24, 57, 74	0
2	D	207/207 (100%)	-0.17	4 (1%) 66 44	5, 23, 61, 76	0
2	F	207/207 (100%)	-0.04	5 (2%) 59 37	10, 31, 63, 82	0
All	All	3087/3147 (98%)	0.56	286 (9%) 14 8	5, 60, 123, 146	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	146	ALA	8.1
1	E	175	TYR	7.3
1	E	343	PRO	7.0
1	E	273	PHE	6.8
1	E	189	VAL	6.8
1	E	339	VAL	6.7
1	E	99	LEU	6.5
1	C	493	VAL	6.0
2	B	519	ALA	6.0
1	E	143	LEU	5.7
1	E	277	ILE	5.7
1	E	338	ILE	5.7
1	E	245	TRP	5.4
1	E	276	PHE	5.4
1	E	335	LEU	5.3
1	E	780	PHE	5.2
1	E	356	LEU	5.0
1	E	126	LEU	4.9
1	E	364	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	155	VAL	4.8
1	E	348	ALA	4.6
1	E	280	PRO	4.6
1	E	154	VAL	4.6
1	C	507	GLY	4.2
1	C	505	VAL	4.2
1	E	781	THR	4.1
1	E	334	LEU	4.1
1	E	188	ILE	4.1
1	E	200	VAL	4.1
1	E	193	ALA	4.1
1	C	323	VAL	4.0
1	E	342	LEU	4.0
1	C	504	LEU	4.0
1	E	151	ILE	4.0
1	C	492	ALA	4.0
2	B	518	LEU	4.0
2	B	521	PRO	4.0
1	E	534	GLY	4.0
1	E	147	LEU	3.9
1	A	495	VAL	3.9
1	E	346	VAL	3.9
1	E	92	LYS	3.8
1	E	368	ALA	3.8
1	E	89	ILE	3.8
1	E	209	VAL	3.7
1	E	196	VAL	3.7
1	E	554	LEU	3.7
1	E	526	GLY	3.6
1	E	109	VAL	3.6
1	E	145	GLN	3.6
1	E	746	VAL	3.5
1	E	17	THR	3.5
1	E	197	LEU	3.5
1	C	530	VAL	3.5
1	C	549	HIS	3.5
1	C	501	LEU	3.5
1	E	21	ASN	3.5
1	C	552	VAL	3.5
1	E	442	VAL	3.4
1	E	349	GLN	3.4
1	E	184	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	770	ALA	3.4
1	E	258	THR	3.4
1	E	525	SER	3.3
1	E	475	ALA	3.3
1	E	128	VAL	3.3
1	E	777	SER	3.3
1	E	275	MET	3.3
1	E	279	ASP	3.3
1	E	784	LEU	3.3
1	E	476	HIS	3.3
1	E	190	SER	3.3
1	E	366	CYS	3.3
2	F	519	ALA	3.3
1	E	93	THR	3.2
1	E	474	THR	3.2
1	C	299	LEU	3.2
1	E	763	THR	3.2
1	C	551	GLY	3.2
1	E	182	VAL	3.2
1	E	420	PRO	3.2
2	D	518	LEU	3.2
1	E	259	ASN	3.2
1	A	420	PRO	3.2
1	E	765	LEU	3.1
1	E	306	VAL	3.1
1	C	498	ALA	3.1
1	E	67	GLY	3.1
1	E	764	PRO	3.1
1	E	39	LEU	3.1
1	E	501	LEU	3.1
1	E	113	SER	3.1
1	E	179	ALA	3.0
1	E	419	VAL	3.0
1	E	86	VAL	3.0
1	E	347	THR	3.0
1	E	79	SER	3.0
1	E	296	ILE	3.0
1	E	492	ALA	3.0
1	C	281	ILE	3.0
1	E	81	MET	3.0
1	E	519	LEU	3.0
1	E	110	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	134	GLY	3.0
1	E	286	THR	3.0
1	E	194	ASP	2.9
1	E	782	GLY	2.9
1	E	216	HIS	2.9
1	C	251	ASN	2.9
1	E	202	VAL	2.9
1	E	493	VAL	2.9
1	A	306	VAL	2.9
1	E	552	VAL	2.9
1	C	557	SER	2.9
1	E	731	VAL	2.9
1	E	20	ARG	2.9
1	E	244	LEU	2.9
1	E	438	MET	2.9
1	E	205	ALA	2.8
1	E	35	LEU	2.8
1	E	97	SER	2.8
1	C	550	ALA	2.8
1	E	201	GLN	2.8
1	E	538	LEU	2.8
1	E	790	GLY	2.8
2	D	519	ALA	2.8
1	E	783	GLU	2.8
1	E	441	PHE	2.7
1	E	365	ASN	2.7
1	E	127	VAL	2.7
1	C	502	PRO	2.7
1	C	291	PHE	2.7
1	E	535	GLU	2.7
1	C	216	HIS	2.7
1	E	443	GLU	2.7
1	E	107	GLY	2.7
1	E	208	THR	2.7
1	C	165	LEU	2.7
1	E	553	PRO	2.7
1	E	796	MET	2.7
1	E	523	SER	2.7
1	E	210	ALA	2.7
1	E	78	TYR	2.7
2	F	518	LEU	2.7
1	E	761	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	260	LYS	2.6
1	C	270	GLU	2.6
1	E	361	ALA	2.6
1	E	743	ILE	2.6
1	E	98	PHE	2.6
1	E	284	LEU	2.6
1	E	747	LEU	2.6
1	C	296	ILE	2.6
1	C	233	PHE	2.6
1	C	327	PHE	2.6
1	E	541	CYS	2.6
1	E	281	ILE	2.6
1	E	379	MET	2.6
1	E	207	GLY	2.6
1	E	100	ILE	2.5
1	E	437	MET	2.5
1	E	90	LYS	2.5
1	E	787	ALA	2.5
1	E	139	THR	2.5
1	E	257	TRP	2.5
1	E	401	PHE	2.5
1	A	216	HIS	2.5
1	C	525	SER	2.5
1	C	554	LEU	2.5
1	E	527	GLU	2.5
1	E	122	THR	2.5
1	E	241	MET	2.5
1	C	300	LEU	2.5
1	C	503	LYS	2.5
1	E	479	LYS	2.5
1	C	277	ILE	2.5
1	E	123	ASP	2.5
1	C	553	PRO	2.5
1	E	444	PRO	2.5
1	C	212	GLY	2.5
1	C	524	GLU	2.4
1	E	116	THR	2.4
1	E	192	TYR	2.4
1	E	73	THR	2.4
1	A	475	ALA	2.4
1	E	367	ILE	2.4
1	E	498	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	520	ALA	2.4
1	C	235	VAL	2.4
1	E	142	VAL	2.4
1	E	204	PRO	2.4
1	E	48	ALA	2.4
1	C	289	MET	2.4
1	E	546	GLU	2.4
1	C	48	ALA	2.3
1	E	87	LYS	2.3
1	C	500	ASP	2.3
1	C	306	VAL	2.3
1	C	764	PRO	2.3
1	E	248	SER	2.3
2	D	521	PRO	2.3
1	E	15	LYS	2.3
1	E	246	GLY	2.3
1	E	551	GLY	2.3
1	E	340	LEU	2.3
2	F	492	ARG	2.3
1	C	258	THR	2.3
1	E	300	LEU	2.3
1	E	247	ASP	2.3
1	E	494	GLU	2.3
1	E	768	VAL	2.3
1	E	331	ALA	2.3
1	A	99	LEU	2.3
1	E	16	VAL	2.3
1	E	360	PRO	2.3
1	E	736	PRO	2.3
1	E	95	GLY	2.3
1	E	547	HIS	2.3
1	C	229	TYR	2.3
1	E	199	ASP	2.3
1	C	536	LEU	2.2
1	A	345	PRO	2.2
1	C	770	ALA	2.2
1	E	421	GLY	2.2
1	E	772	LEU	2.2
1	C	285	PHE	2.2
1	E	178	PHE	2.2
1	C	495	VAL	2.2
1	E	186	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	236	ASP	2.2
1	E	533	THR	2.2
1	E	305	ILE	2.2
1	A	765	LEU	2.2
1	C	761	PRO	2.2
1	E	85	ASP	2.2
1	E	108	HIS	2.2
1	E	19	VAL	2.2
1	C	278	LEU	2.2
1	C	264	ALA	2.2
1	E	735	CYS	2.2
1	E	754	VAL	2.1
1	E	759	GLN	2.1
1	E	33	SER	2.1
2	B	549	GLY	2.1
1	C	263	ASP	2.1
1	E	222	ILE	2.1
1	A	134	GLY	2.1
1	E	23	SER	2.1
1	E	153	PRO	2.1
2	F	459	SER	2.1
1	E	477	ASN	2.1
1	E	2	VAL	2.1
1	E	121	VAL	2.1
1	E	185	VAL	2.1
1	A	237	LYS	2.1
1	C	284	LEU	2.1
1	C	556	ILE	2.1
2	B	520	ALA	2.1
2	D	520	ALA	2.1
1	A	764	PRO	2.1
1	E	187	VAL	2.1
1	C	108	HIS	2.1
1	C	267	LYS	2.1
1	C	288	ILE	2.1
1	C	528	HIS	2.1
1	E	157	ILE	2.1
1	E	536	LEU	2.1
2	B	490	ARG	2.1
1	E	522	MET	2.1
1	E	111	PHE	2.1
1	E	737	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	160	VAL	2.1
1	E	497	ASN	2.1
1	E	238	ALA	2.1
1	E	779	GLY	2.1
1	C	253	LYS	2.0
1	E	82	SER	2.0
1	E	215	LEU	2.0
1	C	93	THR	2.0
1	C	261	ASP	2.0
1	C	237	LYS	2.0
1	E	542	LEU	2.0
1	A	553	PRO	2.0
1	E	308	LYS	2.0
1	E	734	GLN	2.0
1	E	103	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	DDE	E	699	10/21	0.87	0.10	44,48,49,50	0
1	DDE	A	699	10/21	0.91	0.09	40,42,44,45	0
1	DDE	C	699	10/21	0.92	0.09	43,47,48,50	0

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.