



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:55 AM UTC

PDB ID : 1EJ6 / pdb_00001ej6
Title : Reovirus core
Authors : Reinisch, K.M.; Nibert, M.L.; Harrison, S.C.
Deposited on : 2000-02-29
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

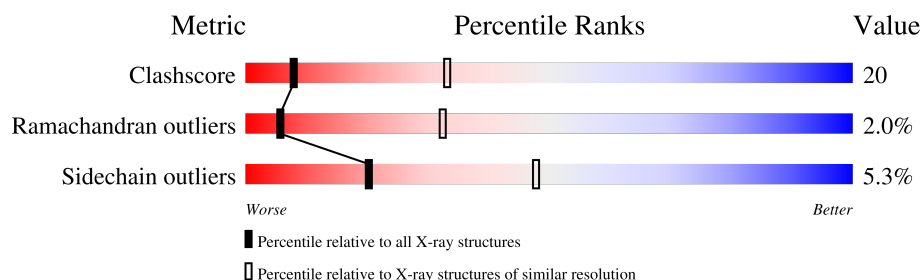
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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))
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1289	
2	B	1275	
2	C	1275	
3	D	418	
3	E	418	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34487 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 LAMBDA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1284	Total	C	N	O	S	0	0	0
			10126	6468	1699	1917	42			

- Molecule 2 is a protein called LAMBDA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1031	Total	C	N	O	S	0	0	0
			8143	5208	1375	1510	50			
2	C	1221	Total	C	N	O	S	0	0	0
			9591	6078	1649	1809	55			

- Molecule 3 is a protein called SIGMA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	417	Total	C	N	O	S	0	0	0
			3313	2092	600	604	17			
3	E	417	Total	C	N	O	S	0	0	0
			3313	2092	600	604	17			

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

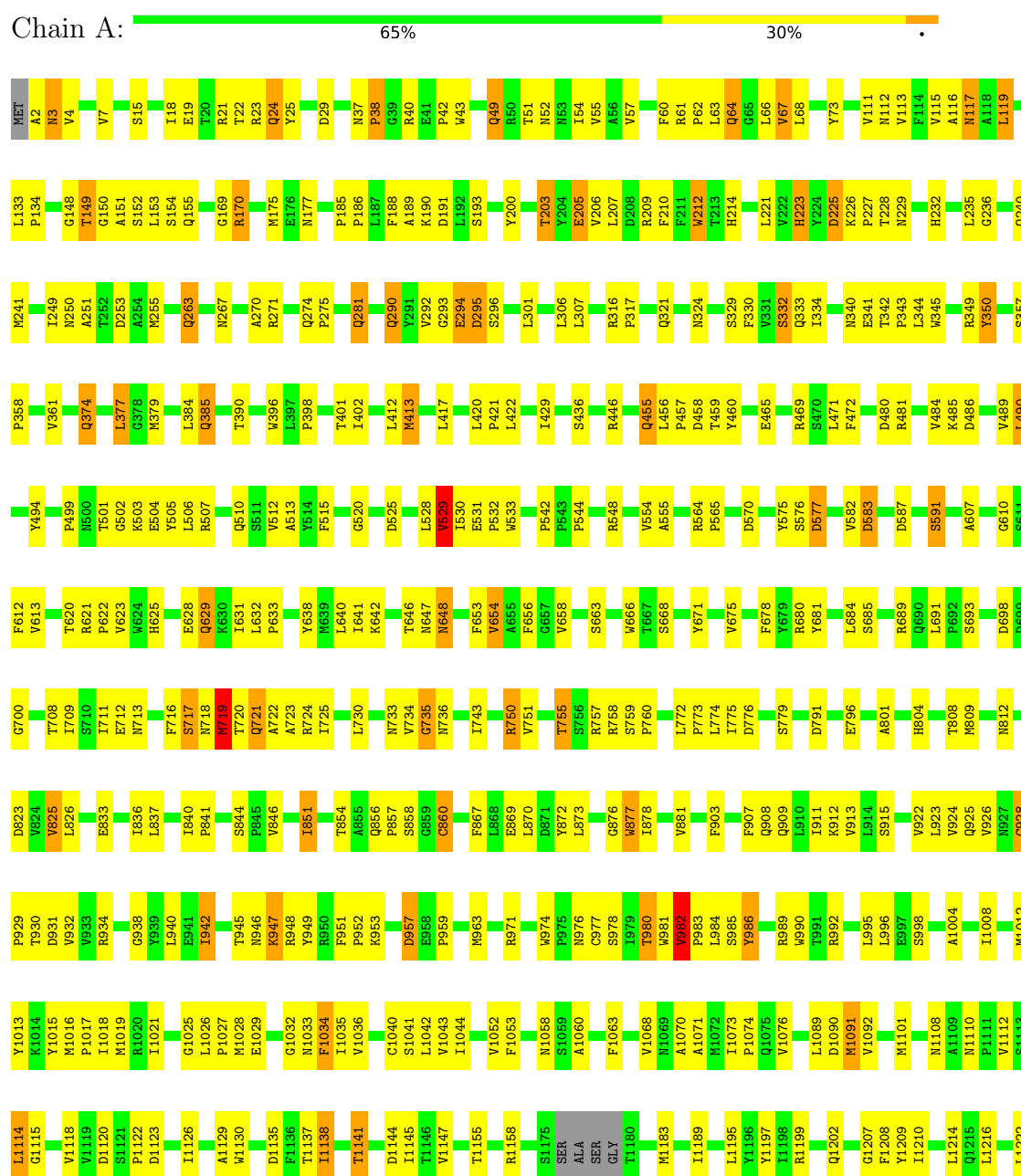
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

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

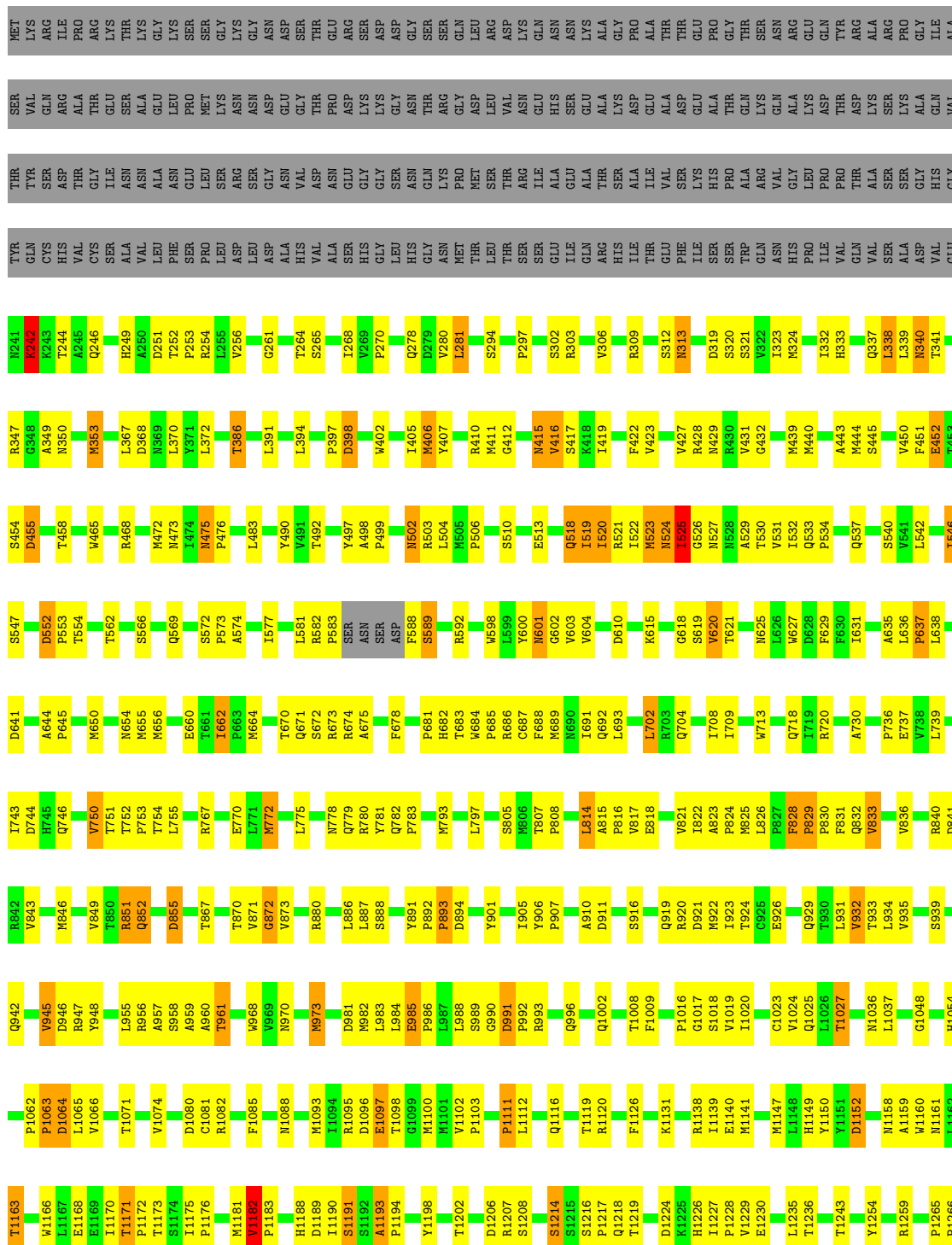
Note EDS was not executed.

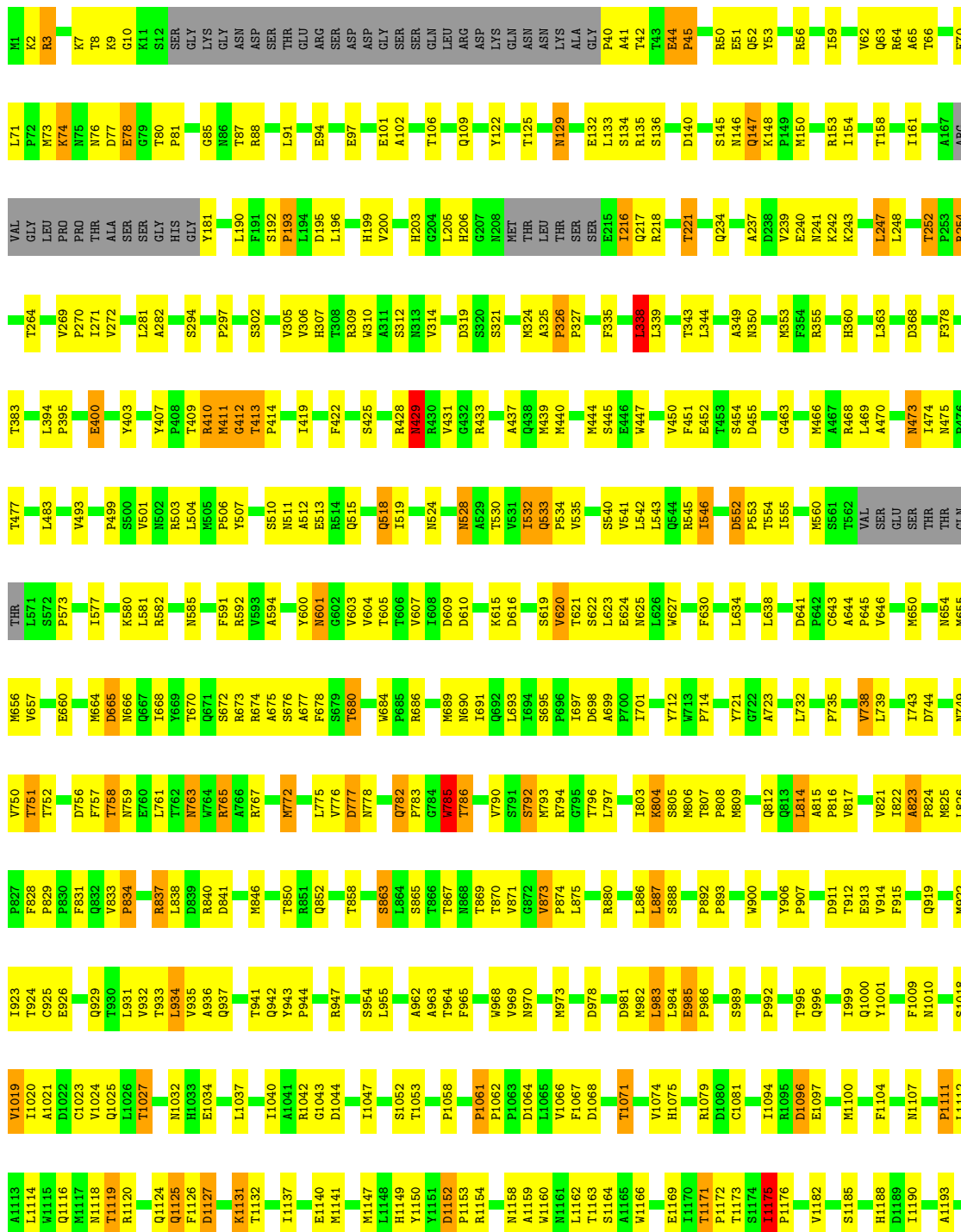
• Molecule 1: LAMBDA2

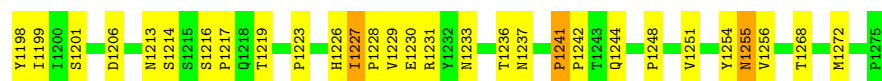




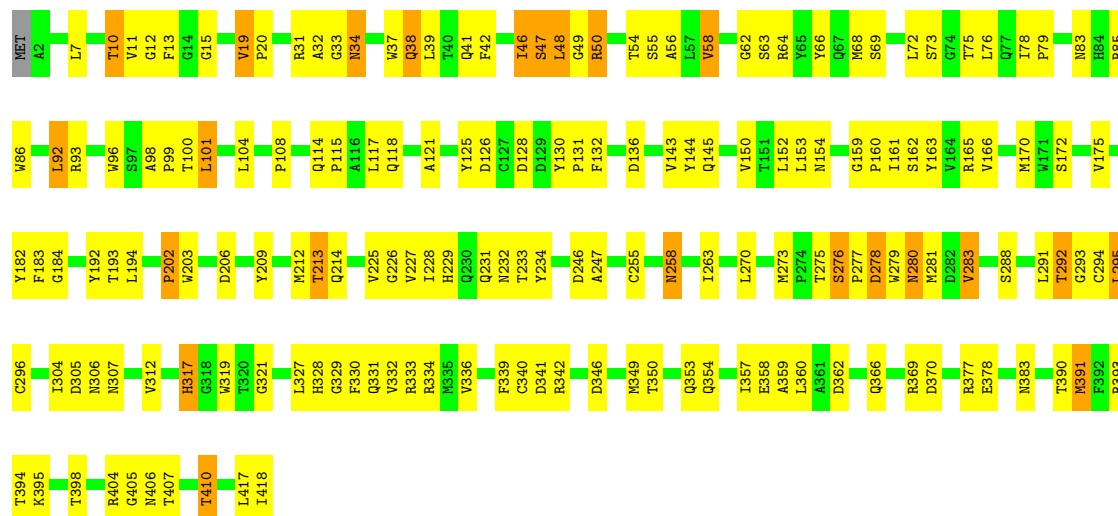
Chain B: 40% 27% 3% 19%



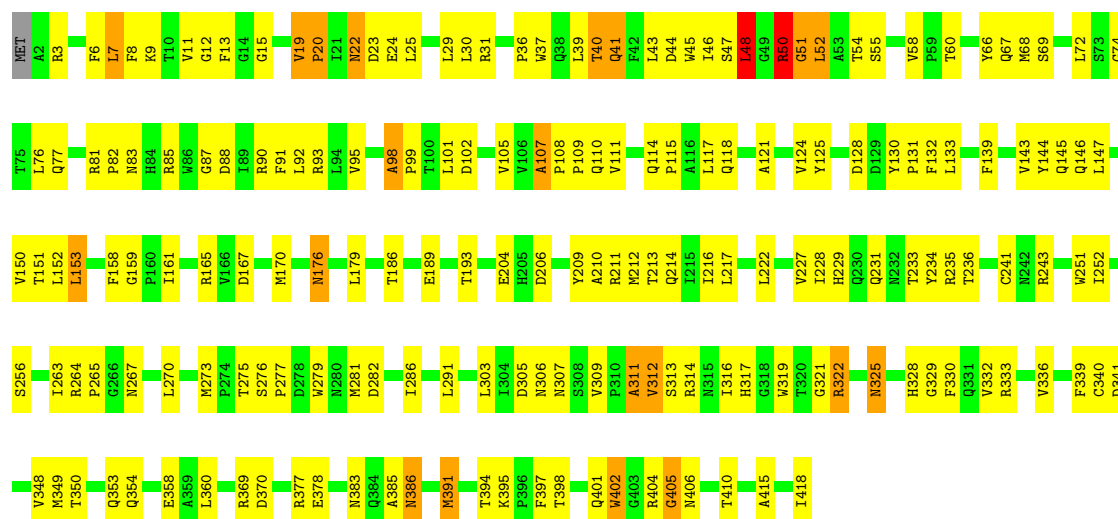




• Molecule 3: SIGMA2



• Molecule 3: SIGMA2



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	1255.00Å 1255.00Å 1255.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60	Depositor
% Data completeness (in resolution range)	88.5 (20.00-3.60)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.208	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	34487	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/10384	0.97	37/14170 (0.3%)
2	B	0.65	0/8363	1.02	47/11454 (0.4%)
2	C	0.62	0/9833	1.03	71/13437 (0.5%)
3	D	0.59	0/3398	0.96	20/4626 (0.4%)
3	E	0.57	1/3398 (0.0%)	0.98	19/4626 (0.4%)
All	All	0.58	1/35376 (0.0%)	1.00	194/48313 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	TRP	NE1-CE2	-5.59	1.31	1.37

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	546	ILE	N-CA-C	-9.38	103.99	113.47
2	B	416	VAL	N-CA-C	-9.05	102.29	111.88
2	C	1097	GLU	N-CA-C	-8.84	102.63	113.50
1	A	390	THR	CA-C-N	8.59	130.57	119.84
1	A	390	THR	C-N-CA	8.59	130.57	119.84
2	C	429	ASN	N-CA-C	8.45	122.69	112.38
2	C	1152	ASP	CA-C-N	8.19	128.97	119.47
2	C	1152	ASP	C-N-CA	8.19	128.97	119.47
1	A	1222	LEU	N-CA-C	7.99	120.14	110.07
2	B	242	LYS	N-CA-C	-7.75	102.16	111.69
1	A	791	ASP	CA-C-N	7.45	127.88	119.83
1	A	791	ASP	C-N-CA	7.45	127.88	119.83
2	C	777	ASP	N-CA-C	7.44	120.10	111.02
2	C	752	THR	CA-C-N	7.44	127.36	119.85
2	C	752	THR	C-N-CA	7.44	127.36	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	SER	N-CA-C	-7.41	104.23	113.20
1	A	982	VAL	N-CA-C	7.41	116.21	108.95
2	C	413	THR	CA-C-N	7.16	126.69	119.24
2	C	413	THR	C-N-CA	7.16	126.69	119.24
3	E	3	ARG	N-CA-C	7.14	120.30	110.24
1	A	796	GLU	N-CA-C	7.06	119.64	111.02
2	C	582	ARG	CA-C-N	6.95	126.56	119.19
2	C	582	ARG	C-N-CA	6.95	126.56	119.19
1	A	1044	ILE	N-CA-C	6.92	115.00	108.15
2	C	888	SER	N-CA-C	6.90	118.99	109.54
2	B	552	ASP	CA-C-N	6.77	127.32	119.47
2	B	552	ASP	C-N-CA	6.77	127.32	119.47
2	B	350	ASN	CA-C-N	6.76	126.55	119.05
2	B	350	ASN	C-N-CA	6.76	126.55	119.05
2	B	828	PHE	CA-C-N	6.73	124.57	119.66
2	B	828	PHE	C-N-CA	6.73	124.57	119.66
2	B	1182	VAL	CA-C-N	6.72	126.64	119.85
2	B	1182	VAL	C-N-CA	6.72	126.64	119.85
3	D	58	VAL	CA-C-N	6.69	126.29	119.19
3	D	58	VAL	C-N-CA	6.69	126.29	119.19
2	C	247	LEU	N-CA-C	6.69	120.42	109.72
3	D	47	SER	N-CA-C	6.68	119.38	111.02
3	D	38	GLN	N-CA-C	6.58	122.45	113.37
1	A	37	ASN	CA-C-N	6.55	128.03	119.84
1	A	37	ASN	C-N-CA	6.55	128.03	119.84
3	E	50	ARG	N-CA-C	-6.54	103.55	113.89
2	C	314	VAL	N-CA-C	6.50	118.52	109.29
2	C	519	ILE	N-CA-C	-6.50	103.91	111.00
2	B	752	THR	CA-C-N	6.47	127.93	119.84
2	B	752	THR	C-N-CA	6.47	127.93	119.84
3	E	159	GLY	CA-C-N	6.45	128.16	120.23
3	E	159	GLY	C-N-CA	6.45	128.16	120.23
3	E	58	VAL	CA-C-N	6.39	125.88	119.24
3	E	58	VAL	C-N-CA	6.39	125.88	119.24
2	B	1152	ASP	CA-C-N	6.32	126.80	119.47
2	B	1152	ASP	C-N-CA	6.32	126.80	119.47
3	E	107	ALA	CA-C-N	6.30	124.19	119.66
3	E	107	ALA	C-N-CA	6.30	124.19	119.66
1	A	1114	LEU	N-CA-C	-6.29	100.02	109.96
2	B	294	SER	CA-C-N	6.25	125.82	119.19
2	B	294	SER	C-N-CA	6.25	125.82	119.19
2	C	873	VAL	CA-C-N	6.24	126.46	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	873	VAL	C-N-CA	6.24	126.46	119.90
2	B	872	GLY	N-CA-C	6.24	119.89	111.72
2	C	383	THR	N-CA-C	-6.22	101.92	109.83
3	E	348	VAL	N-CA-C	-6.22	107.44	113.53
1	A	64	GLN	N-CA-C	-6.21	105.28	112.92
2	B	662	ILE	N-CA-C	6.19	114.71	107.84
1	A	212	TRP	N-CA-C	-6.17	104.63	111.36
2	B	888	SER	N-CA-C	6.17	117.84	110.44
3	E	15	GLY	N-CA-C	-6.14	106.68	115.64
1	A	925	GLN	N-CA-C	-6.09	100.82	109.96
2	C	758	THR	N-CA-C	-6.08	104.93	112.90
2	B	945	VAL	N-CA-C	6.06	115.10	107.70
3	D	292	THR	N-CA-C	-6.05	105.00	112.38
1	A	776	ASP	CA-C-N	6.04	127.40	119.84
1	A	776	ASP	C-N-CA	6.04	127.40	119.84
1	A	858	SER	N-CA-C	6.03	120.32	111.34
3	E	36	PRO	N-CA-C	-6.00	108.44	114.68
2	C	1169	GLU	N-CA-C	6.00	119.65	112.93
2	C	1193	ALA	CA-C-N	6.00	126.01	119.89
2	C	1193	ALA	C-N-CA	6.00	126.01	119.89
1	A	15	SER	CA-C-N	5.99	125.95	119.78
1	A	15	SER	C-N-CA	5.99	125.95	119.78
3	D	319	TRP	N-CA-C	5.97	120.12	112.12
2	C	1233	ASN	N-CA-C	5.89	117.39	110.97
1	A	40	ARG	N-CA-C	5.87	116.82	108.54
2	C	1227	ILE	CA-C-N	5.86	127.17	119.84
2	C	1227	ILE	C-N-CA	5.86	127.17	119.84
2	B	429	ASN	N-CA-C	5.84	123.25	110.80
3	E	98	ALA	CA-C-N	5.84	125.31	119.24
3	E	98	ALA	C-N-CA	5.84	125.31	119.24
2	C	532	ILE	CB-CA-C	-5.83	104.28	111.92
2	C	269	VAL	N-CA-C	5.80	114.28	107.84
2	B	988	LEU	N-CA-C	5.77	119.79	112.87
1	A	240	GLN	N-CA-C	5.76	117.83	109.07
2	C	738	VAL	N-CA-C	5.75	117.88	108.97
3	D	283	VAL	N-CA-C	5.73	117.15	110.62
2	C	252	THR	CA-C-N	5.71	126.19	120.14
2	C	252	THR	C-N-CA	5.71	126.19	120.14
2	B	1111	PRO	N-CA-C	-5.70	101.57	111.32
1	A	577	ASP	N-CA-C	-5.68	106.15	112.57
1	A	18	ILE	N-CA-C	5.68	116.06	108.11
3	D	108	PRO	N-CA-C	-5.65	104.53	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	395	LYS	CA-C-N	5.61	125.54	119.76
3	D	395	LYS	C-N-CA	5.61	125.54	119.76
2	C	1131	LYS	N-CA-C	5.60	117.08	110.97
2	B	519	ILE	N-CA-C	-5.60	105.39	110.82
3	E	102	ASP	N-CA-C	5.60	117.83	111.11
2	C	723	ALA	CA-C-N	5.58	126.81	119.84
2	C	723	ALA	C-N-CA	5.58	126.81	119.84
2	C	783	PRO	N-CA-C	-5.55	101.03	112.47
3	D	296	CYS	N-CA-C	5.53	118.07	111.71
1	A	49	GLN	N-CA-C	5.52	119.50	112.87
2	C	1061	PRO	CA-C-N	5.52	126.06	120.38
2	C	1061	PRO	C-N-CA	5.52	126.06	120.38
2	B	957	ALA	N-CA-C	5.51	118.53	109.76
2	B	1098	THR	N-CA-C	-5.51	105.92	113.30
2	C	1125	GLN	N-CA-C	5.47	118.16	111.82
2	C	1111	PRO	N-CA-C	-5.46	101.98	111.32
2	B	1193	ALA	CA-C-N	5.45	126.66	119.84
2	B	1193	ALA	C-N-CA	5.45	126.66	119.84
3	E	319	TRP	N-CA-C	5.45	119.31	111.02
2	C	1237	ASN	CA-C-N	5.45	125.53	119.32
2	C	1237	ASN	C-N-CA	5.45	125.53	119.32
2	C	193	PRO	N-CA-C	-5.45	105.95	113.53
2	B	445	SER	N-CA-C	-5.45	101.59	110.20
3	D	19	VAL	CA-C-N	5.43	126.63	119.84
3	D	19	VAL	C-N-CA	5.43	126.63	119.84
1	A	881	VAL	N-CA-C	5.42	116.58	109.58
2	C	680	THR	CA-C-N	5.42	125.24	119.28
2	C	680	THR	C-N-CA	5.42	125.24	119.28
2	B	1126	PHE	N-CA-C	5.40	119.87	113.12
2	C	125	THR	N-CA-C	-5.40	102.53	110.52
1	A	502	GLY	N-CA-C	-5.39	107.54	115.30
1	A	629	GLN	N-CA-C	5.37	117.21	111.36
2	C	996	GLN	N-CA-C	5.35	117.22	108.55
1	A	576	SER	N-CA-C	5.35	118.45	107.69
3	D	159	GLY	CA-C-N	5.34	125.51	119.90
3	D	159	GLY	C-N-CA	5.34	125.51	119.90
2	B	475	ASN	CA-C-N	5.33	126.51	119.84
2	B	475	ASN	C-N-CA	5.33	126.51	119.84
2	C	44	GLU	CA-C-N	5.33	126.03	120.12
2	C	44	GLU	C-N-CA	5.33	126.03	120.12
2	B	781	TYR	N-CA-C	-5.30	108.57	114.62
2	C	786	THR	N-CA-C	5.29	116.73	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	276	SER	CA-C-N	5.29	125.60	119.47
3	D	276	SER	C-N-CA	5.29	125.60	119.47
2	C	71	LEU	CA-C-N	5.28	125.19	119.85
2	C	71	LEU	C-N-CA	5.28	125.19	119.85
3	D	136	ASP	CA-C-N	5.28	126.43	119.84
3	D	136	ASP	C-N-CA	5.28	126.43	119.84
2	B	405	ILE	N-CA-C	-5.26	105.32	113.16
2	C	1164	SER	N-CA-C	-5.26	105.19	111.03
2	B	398	ASP	N-CA-C	-5.25	104.89	111.92
2	B	1097	GLU	N-CA-C	-5.25	106.92	113.38
3	E	309	VAL	N-CA-C	5.24	113.66	107.84
2	C	552	ASP	CA-C-N	5.23	125.29	119.32
2	C	552	ASP	C-N-CA	5.23	125.29	119.32
3	E	19	VAL	CA-C-N	5.23	126.38	119.84
3	E	19	VAL	C-N-CA	5.23	126.38	119.84
2	B	829	PRO	CA-C-N	5.21	125.21	119.89
2	B	829	PRO	C-N-CA	5.21	125.21	119.89
2	C	428	ARG	N-CA-C	5.21	116.65	111.07
2	C	74	LYS	N-CA-C	5.21	117.78	110.23
2	C	735	PRO	CA-C-N	5.21	125.25	119.32
2	C	735	PRO	C-N-CA	5.21	125.25	119.32
2	C	45	PRO	N-CA-C	5.20	120.44	114.20
1	A	860	CYS	N-CA-C	5.18	118.86	112.54
2	B	520	ILE	N-CA-C	-5.18	104.92	110.36
2	B	323	ILE	N-CA-C	5.18	115.31	107.75
3	D	15	GLY	N-CA-C	-5.17	107.66	115.32
2	B	956	ARG	N-CA-C	-5.16	100.67	108.67
2	B	991	ASP	CA-C-N	5.16	127.29	121.04
2	B	991	ASP	C-N-CA	5.16	127.29	121.04
1	A	529	VAL	CB-CA-C	-5.15	105.27	112.02
1	A	67	VAL	N-CA-C	5.15	118.09	113.10
2	C	148	LYS	CA-C-N	5.14	125.14	119.90
2	C	148	LYS	C-N-CA	5.14	125.14	119.90
2	C	712	TYR	N-CA-C	5.12	121.29	113.61
2	C	1137	ILE	N-CA-C	5.11	115.27	108.11
2	C	326	PRO	CA-C-N	5.10	126.22	119.84
2	C	326	PRO	C-N-CA	5.10	126.22	119.84
2	B	1062	PRO	CA-C-N	5.10	126.21	119.84
2	B	1062	PRO	C-N-CA	5.10	126.21	119.84
1	A	504	GLU	N-CA-C	5.08	117.47	110.35
2	C	804	LYS	N-CA-C	5.08	117.75	110.68
2	C	1241	PRO	CA-C-N	5.08	125.11	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1241	PRO	C-N-CA	5.08	125.11	119.32
2	C	785	TRP	N-CA-C	-5.06	97.64	107.62
2	B	910	ALA	N-CA-C	-5.06	105.81	112.94
1	A	1271	SER	CA-C-N	5.03	125.31	119.47
1	A	1271	SER	C-N-CA	5.03	125.31	119.47
1	A	942	ILE	N-CA-C	5.03	116.20	108.71
1	A	825	VAL	N-CA-C	5.02	116.58	108.85
2	B	892	PRO	N-CA-C	-5.02	105.65	110.47
3	E	153	LEU	N-CA-C	-5.02	107.14	114.12
2	C	109	GLN	N-CA-C	-5.01	105.27	111.33
2	C	892	PRO	N-CA-C	-5.01	104.59	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10126	0	9906	332	0
2	B	8143	0	8063	333	0
2	C	9591	0	9453	394	0
3	D	3313	0	3215	151	0
3	E	3313	0	3215	162	0
4	C	1	0	0	0	0
All	All	34487	0	33852	1347	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1347) 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)
2:C:1171:THR:HG22	2:C:1173:THR:H	1.08	1.16
1:A:1138:ILE:HD12	1:A:1138:ILE:H	1.21	1.05
2:C:106:THR:HG22	2:C:122:TYR:H	1.15	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:HG22	1:A:151:ALA:H	1.22	1.01
2:B:1171:THR:HG22	2:B:1173:THR:H	1.22	1.01
1:A:851:ILE:HD12	1:A:851:ILE:H	1.26	0.98
3:E:229:HIS:HD2	3:E:231:GLN:H	1.11	0.97
2:B:691:ILE:HD12	2:B:691:ILE:H	1.30	0.96
3:D:258:ASN:HD22	3:D:258:ASN:H	1.01	0.96
3:D:209:TYR:O	3:D:213:THR:HG22	1.65	0.96
1:A:750:ARG:HH11	1:A:750:ARG:HG2	1.26	0.96
1:A:825:VAL:HB	1:A:846:VAL:HG12	1.45	0.96
1:A:456:LEU:HD12	1:A:457:PRO:HD2	1.46	0.94
3:E:47:SER:HB2	3:E:50:ARG:HH22	1.33	0.94
1:A:263:GLN:HG2	1:A:281:GLN:HB2	1.47	0.94
2:C:691:ILE:HD12	2:C:691:ILE:H	1.32	0.93
3:E:41:GLN:HE21	3:E:41:GLN:HA	1.35	0.92
2:C:439:MET:HE1	3:E:193:THR:HB	1.51	0.91
3:D:258:ASN:HD22	3:D:258:ASN:N	1.66	0.90
2:B:1112:LEU:HG	2:B:1116:GLN:HE21	1.38	0.89
3:E:306:ASN:HB3	3:E:314:ARG:HD3	1.55	0.89
3:E:179:LEU:HD23	3:E:212:MET:HE3	1.55	0.88
2:C:1171:THR:HG22	2:C:1173:THR:N	1.89	0.87
2:C:560:MET:HE1	2:C:796:THR:HG23	1.56	0.86
2:C:601:ASN:ND2	2:C:833:VAL:H	1.73	0.86
2:B:439:MET:HE2	3:D:184:GLY:HA2	1.56	0.86
1:A:306:LEU:HD23	1:A:344:LEU:HB3	1.57	0.86
2:B:1168:GLU:HB3	2:C:50:ARG:HG3	1.56	0.85
2:B:522:ILE:O	2:B:525:ILE:HG23	1.76	0.85
2:C:1171:THR:HG23	2:C:1172:PRO:HD2	1.58	0.85
2:C:533:GLN:HB3	2:C:534:PRO:HD3	1.59	0.84
2:C:2:LYS:HG2	2:C:3:ARG:H	1.44	0.83
2:B:1171:THR:HG22	2:B:1173:THR:N	1.93	0.83
3:D:258:ASN:H	3:D:258:ASN:ND2	1.76	0.83
2:B:1096:ASP:HB3	2:B:1100:MET:H	1.44	0.82
2:B:823:ALA:HA	2:B:826:LEU:HD23	1.60	0.82
1:A:153:LEU:HB3	1:A:155:GLN:HG2	1.60	0.82
2:B:532:ILE:HG12	2:B:604:VAL:HG21	1.61	0.81
3:E:325:ASN:N	3:E:325:ASN:HD22	1.78	0.81
2:B:339:LEU:HB2	2:B:353:MET:HG3	1.62	0.81
2:B:1229:VAL:HG13	2:B:1236:THR:HG21	1.61	0.80
2:C:625:ASN:HB3	2:C:655:MET:HE3	1.64	0.80
3:D:340:CYS:HA	3:D:349:MET:HE1	1.62	0.80
2:B:527:ASN:HA	2:B:873:VAL:HG13	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:ASN:C	1:A:648:ASN:HD22	1.90	0.79
1:A:1138:ILE:H	1:A:1138:ILE:CD1	1.96	0.79
2:C:106:THR:CG2	2:C:122:TYR:H	1.95	0.78
1:A:24:GLN:H	1:A:24:GLN:CD	1.89	0.78
2:B:610:ASP:HB2	2:C:786:THR:HG21	1.66	0.78
1:A:455:GLN:HG2	1:A:621:ARG:HG3	1.65	0.77
3:E:37:TRP:CZ3	3:E:143:VAL:HG13	2.19	0.77
2:C:528:ASN:C	2:C:528:ASN:HD22	1.90	0.77
2:C:528:ASN:HD21	2:C:530:THR:HB	1.50	0.77
2:C:1023:CYS:O	2:C:1027:THR:HG23	1.85	0.77
2:C:1152:ASP:OD1	2:C:1154:ARG:HG2	1.84	0.77
3:D:7:LEU:HD11	3:D:317:HIS:HB3	1.66	0.77
2:C:623:LEU:HD13	2:C:793:MET:HE1	1.67	0.76
2:B:265:SER:OG	2:B:458:THR:HG21	1.85	0.76
2:C:106:THR:HG22	2:C:122:TYR:N	1.96	0.76
3:D:50:ARG:HG3	3:D:50:ARG:HH11	1.49	0.75
2:B:603:VAL:HG23	2:B:604:VAL:HG23	1.69	0.75
3:E:229:HIS:CD2	3:E:231:GLN:H	2.01	0.75
2:B:510:SER:OG	2:B:513:GLU:HG3	1.86	0.75
1:A:708:THR:HB	1:A:755:THR:HG23	1.69	0.75
2:C:1079:ARG:HG2	2:C:1079:ARG:HH11	1.52	0.74
1:A:1068:VAL:HG11	1:A:1076:VAL:O	1.87	0.74
3:E:8:PHE:HA	3:E:151:THR:HG21	1.70	0.74
2:C:254:ARG:HH11	2:C:254:ARG:HB3	1.52	0.74
1:A:290:GLN:H	1:A:290:GLN:NE2	1.83	0.74
2:B:662:ILE:HG13	2:B:664:MET:HE3	1.68	0.74
2:C:433:ARG:HA	2:C:450:VAL:HG12	1.70	0.74
3:E:81:ARG:HB3	3:E:82:PRO:HD2	1.69	0.74
1:A:721:GLN:O	1:A:725:ILE:HG12	1.87	0.74
3:D:328:HIS:HB3	3:D:410:THR:HB	1.70	0.74
3:E:383:ASN:HD21	3:E:391:MET:H	1.33	0.74
1:A:750:ARG:HG2	1:A:750:ARG:NH1	1.97	0.74
2:B:822:ILE:HG22	2:B:826:LEU:HD21	1.70	0.74
3:E:51:GLY:O	3:E:52:LEU:HB2	1.88	0.73
3:E:349:MET:HE3	3:E:354:GLN:HB2	1.69	0.73
3:E:22:ASN:C	3:E:22:ASN:HD22	1.95	0.73
3:E:47:SER:CB	3:E:50:ARG:HH22	2.00	0.73
1:A:175:MET:HE3	1:A:175:MET:HA	1.69	0.73
3:D:273:MET:CE	3:D:327:LEU:HD13	2.19	0.73
3:E:263:ILE:HD13	3:E:418:ILE:HG23	1.71	0.73
2:B:278:GLN:HE21	2:B:281:LEU:H	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:893:PRO:HG2	2:B:894:ASP:H	1.53	0.72
3:D:38:GLN:HB2	3:D:68:MET:HE3	1.71	0.72
2:B:553:PRO:HB3	2:B:583:PRO:HB2	1.69	0.72
2:C:413:THR:N	2:C:414:PRO:HD3	2.04	0.72
2:C:815:ALA:HB3	2:C:816:PRO:HD3	1.69	0.72
1:A:878:ILE:HG13	1:A:913:VAL:HG12	1.72	0.72
2:B:340:ASN:N	2:B:340:ASN:HD22	1.86	0.72
1:A:1126:ILE:HG13	1:A:1147:VAL:CG2	2.20	0.72
1:A:149:THR:HG22	1:A:151:ALA:N	2.01	0.72
2:B:280:VAL:HG23	2:B:281:LEU:N	2.03	0.72
2:C:607:VAL:HG12	2:C:641:ASP:HB2	1.72	0.71
2:C:62:VAL:O	2:C:66:THR:HG23	1.89	0.71
2:C:601:ASN:HD21	2:C:833:VAL:H	1.35	0.71
2:B:650:MET:HE2	2:B:678:PHE:CZ	2.25	0.71
2:B:278:GLN:HE21	2:B:280:VAL:HG22	1.55	0.71
3:E:340:CYS:CB	3:E:349:MET:HE1	2.19	0.71
2:C:644:ALA:HB3	2:C:645:PRO:HD3	1.71	0.71
3:D:46:ILE:HD11	3:D:283:VAL:HG13	1.72	0.70
2:C:870:THR:HG22	2:C:871:VAL:H	1.56	0.70
3:D:276:SER:OG	3:D:332:VAL:HG23	1.91	0.70
2:C:74:LYS:HD3	2:C:530:THR:HG22	1.71	0.70
1:A:642:LYS:HZ1	1:A:648:ASN:HD21	1.39	0.70
1:A:720:THR:HG22	1:A:723:ALA:HB3	1.72	0.70
2:B:552:ASP:OD1	2:B:554:THR:HG23	1.92	0.70
2:C:912:THR:OG1	2:C:914:VAL:HG23	1.90	0.70
3:D:270:LEU:C	3:D:270:LEU:HD12	2.16	0.70
2:C:154:ILE:O	2:C:158:THR:HG23	1.92	0.70
1:A:719:MET:HA	1:A:719:MET:HE2	1.73	0.70
3:E:176:ASN:C	3:E:176:ASN:HD22	2.00	0.70
1:A:963:MET:HG3	1:A:981:TRP:CZ2	2.27	0.70
2:B:1112:LEU:HD22	2:B:1141:MET:HE2	1.72	0.70
1:A:642:LYS:NZ	1:A:648:ASN:HD21	1.90	0.70
2:B:278:GLN:HE21	2:B:280:VAL:CG2	2.05	0.69
2:B:320:SER:O	2:B:368:ASP:HB2	1.92	0.69
2:C:400:GLU:HA	2:C:403:TYR:CD2	2.26	0.69
2:C:528:ASN:ND2	2:C:530:THR:HB	2.06	0.69
1:A:292:VAL:HG13	1:A:296:SER:OG	1.92	0.69
2:B:674:ARG:H	2:B:674:ARG:HD3	1.56	0.69
2:B:468:ARG:HB2	2:B:1019:VAL:HG11	1.73	0.69
2:C:192:SER:HB3	2:C:195:ASP:HB2	1.75	0.69
3:D:360:LEU:C	3:D:360:LEU:HD23	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:LEU:N	1:A:633:PRO:HD2	2.08	0.69
2:B:339:LEU:HB2	2:B:353:MET:CG	2.21	0.69
2:B:1023:CYS:O	2:B:1027:THR:HG23	1.92	0.69
3:E:22:ASN:ND2	3:E:25:LEU:H	1.91	0.69
2:B:961:THR:HG22	2:C:893:PRO:O	1.92	0.68
2:B:1171:THR:HG23	2:B:1172:PRO:HD2	1.74	0.68
2:C:2:LYS:O	2:C:3:ARG:HB2	1.93	0.68
2:C:605:THR:HG21	2:C:870:THR:HG21	1.75	0.68
1:A:980:THR:HB	1:A:1115:GLY:HA2	1.73	0.68
2:B:280:VAL:HG23	2:B:281:LEU:H	1.59	0.68
3:E:22:ASN:HD21	3:E:25:LEU:H	1.41	0.68
2:C:218:ARG:HH21	2:C:239:VAL:HG21	1.56	0.68
2:B:242:LYS:H	2:B:242:LYS:HD2	1.57	0.68
2:B:278:GLN:NE2	2:B:280:VAL:HG22	2.07	0.68
1:A:374:GLN:CD	1:A:374:GLN:H	1.99	0.68
1:A:385:GLN:HE21	1:A:385:GLN:HA	1.58	0.68
2:C:1171:THR:HG23	2:C:1172:PRO:CD	2.23	0.68
2:C:94:GLU:HB3	2:C:133:LEU:HD22	1.74	0.68
2:B:1188:HIS:O	2:B:1190:ILE:HG23	1.94	0.68
1:A:1063:PHE:HD2	1:A:1073:ILE:HD12	1.58	0.68
2:C:483:LEU:HB2	2:C:493:VAL:HG21	1.75	0.68
2:B:503:ARG:HD3	2:B:1265:PRO:HG3	1.76	0.68
2:B:1217:PRO:HG2	2:B:1218:GLN:OE1	1.94	0.68
2:C:620:VAL:HG11	2:C:656:MET:HE2	1.76	0.68
3:E:340:CYS:HB3	3:E:349:MET:HE1	1.76	0.68
2:C:666:ASN:OD1	2:C:668:ILE:HB	1.93	0.67
2:B:851:ARG:HA	2:B:996:GLN:O	1.94	0.67
2:C:237:ALA:HA	2:C:247:LEU:HD22	1.75	0.67
1:A:700:GLY:HA2	1:A:758:ARG:NH2	2.10	0.67
2:C:1158:ASN:C	2:C:1158:ASN:HD22	2.02	0.67
3:E:209:TYR:O	3:E:213:THR:HG23	1.95	0.67
2:C:305:VAL:HG13	2:C:324:MET:HE2	1.76	0.67
1:A:1145:ILE:HG22	1:A:1147:VAL:HG23	1.77	0.67
2:C:218:ARG:HH21	2:C:239:VAL:CG2	2.07	0.67
2:C:763:ASN:ND2	2:C:767:ARG:HG2	2.10	0.67
3:E:386:ASN:N	3:E:386:ASN:HD22	1.93	0.67
2:B:851:ARG:HG3	2:B:851:ARG:HH11	1.58	0.67
3:D:114:GLN:HB3	3:D:115:PRO:HD2	1.77	0.67
3:E:276:SER:OG	3:E:332:VAL:HG23	1.95	0.67
3:E:270:LEU:HD12	3:E:270:LEU:C	2.20	0.67
1:A:494:TYR:CD2	1:A:542:PRO:HD2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:MET:O	1:A:417:LEU:HD12	1.96	0.66
2:B:303:ARG:HH11	2:B:1208:SER:HB3	1.59	0.66
2:C:321:SER:HA	2:C:368:ASP:OD1	1.95	0.66
1:A:909:GLN:O	1:A:913:VAL:HG23	1.95	0.66
1:A:1108:ASN:HD21	1:A:1110:ASN:HD21	1.42	0.66
1:A:1242:GLU:HB2	1:A:1247:ILE:HD11	1.77	0.66
2:C:412:GLY:C	2:C:414:PRO:HD3	2.21	0.66
3:E:222:LEU:HB3	3:E:228:ILE:HG12	1.76	0.66
3:E:386:ASN:N	3:E:386:ASN:ND2	2.42	0.66
2:B:867:THR:HG22	2:B:867:THR:O	1.96	0.66
2:C:271:ILE:HG22	2:C:272:VAL:HG23	1.78	0.66
3:E:210:ALA:O	3:E:214:GLN:HG3	1.96	0.66
1:A:506:LEU:HD22	1:A:510:GLN:HE22	1.61	0.66
3:E:9:LYS:H	3:E:151:THR:HG22	1.61	0.66
1:A:907:PHE:HZ	1:A:1019:MET:HE1	1.62	0.65
3:D:340:CYS:CA	3:D:349:MET:HE1	2.26	0.65
1:A:857:PRO:HB2	1:A:860:CYS:SG	2.37	0.65
1:A:401:THR:HG22	1:A:774:LEU:O	1.95	0.65
1:A:582:VAL:HG13	1:A:587:ASP:HB2	1.78	0.65
1:A:851:ILE:HD12	1:A:851:ILE:N	2.06	0.65
1:A:621:ARG:HB2	1:A:622:PRO:HD3	1.79	0.65
2:B:353:MET:SD	2:B:955:LEU:HD23	2.36	0.65
2:B:823:ALA:HB3	2:B:824:PRO:HD3	1.78	0.65
2:C:221:THR:HB	2:C:234:GLN:HB2	1.78	0.65
3:D:288:SER:O	3:D:292:THR:HG23	1.96	0.65
1:A:1063:PHE:CD2	1:A:1073:ILE:HD12	2.31	0.65
3:E:328:HIS:HB3	3:E:410:THR:HB	1.79	0.65
1:A:1108:ASN:HD21	1:A:1110:ASN:ND2	1.93	0.65
2:B:682:HIS:CD2	2:C:778:ASN:HB3	2.31	0.65
2:C:474:ILE:HD12	2:C:507:TYR:HB2	1.78	0.65
2:C:623:LEU:CD1	2:C:793:MET:HE1	2.26	0.65
1:A:1068:VAL:HG13	1:A:1076:VAL:HB	1.78	0.65
2:B:252:THR:HG21	2:B:916:SER:HB3	1.78	0.65
2:B:532:ILE:HG12	2:B:604:VAL:CG2	2.26	0.65
3:D:383:ASN:HD21	3:D:391:MET:H	1.43	0.65
1:A:1138:ILE:HD12	1:A:1138:ILE:N	2.05	0.65
2:C:622:SER:HB3	2:C:625:ASN:HD22	1.61	0.65
2:B:1112:LEU:HG	2:B:1116:GLN:NE2	2.10	0.65
2:C:1124:GLN:HG3	2:C:1125:GLN:NE2	2.11	0.65
3:E:39:LEU:C	3:E:41:GLN:H	2.05	0.65
1:A:613:VAL:HG22	1:A:654:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:PRO:C	1:A:984:LEU:HD12	2.21	0.64
1:A:1019:MET:CE	1:A:1021:ILE:HD11	2.26	0.64
2:B:815:ALA:HB3	2:B:816:PRO:HD3	1.80	0.64
2:C:690:ASN:HB3	2:C:693:LEU:HD12	1.78	0.64
2:C:937:GLN:HA	2:C:947:ARG:HH21	1.61	0.64
1:A:290:GLN:H	1:A:290:GLN:HE21	1.42	0.64
3:E:90:ARG:HD3	3:E:111:VAL:HG12	1.79	0.64
3:E:227:VAL:HG21	3:E:415:ALA:HA	1.78	0.64
2:C:765:ARG:HG3	2:C:765:ARG:HH11	1.63	0.64
1:A:903:PHE:CE2	1:A:926:VAL:HG13	2.32	0.64
3:E:11:VAL:HG22	3:E:12:GLY:N	2.12	0.64
2:B:313:ASN:C	2:B:313:ASN:HD22	2.04	0.64
2:B:527:ASN:HA	2:B:873:VAL:CG1	2.27	0.64
1:A:62:PRO:O	1:A:63:LEU:HB2	1.98	0.64
2:B:468:ARG:HD2	2:B:468:ARG:O	1.98	0.64
2:C:528:ASN:C	2:C:528:ASN:ND2	2.54	0.64
3:D:165:ARG:HH11	3:D:214:GLN:HE22	1.44	0.64
3:D:258:ASN:N	3:D:258:ASN:ND2	2.39	0.64
3:D:406:ASN:O	3:D:410:THR:HG23	1.98	0.64
1:A:1074:PRO:HG2	1:A:1092:VAL:O	1.98	0.63
2:B:750:VAL:HG12	2:B:751:THR:H	1.64	0.63
2:B:982:MET:HB3	2:B:985:GLU:HG3	1.79	0.63
3:D:11:VAL:HG22	3:D:12:GLY:N	2.12	0.63
2:B:840:ARG:HA	2:B:843:VAL:HG23	1.80	0.63
1:A:720:THR:CG2	1:A:723:ALA:HB3	2.28	0.63
2:C:122:TYR:CE2	2:C:875:LEU:HD13	2.34	0.63
3:D:334:ARG:HB3	3:D:407:THR:HG21	1.81	0.63
1:A:25:TYR:CZ	1:A:61:ARG:HD3	2.34	0.63
2:C:473:ASN:HD22	2:C:474:ILE:H	1.45	0.63
1:A:153:LEU:HB3	1:A:155:GLN:CG	2.28	0.63
1:A:1126:ILE:HG13	1:A:1147:VAL:HG22	1.80	0.62
2:B:416:VAL:HG12	2:B:416:VAL:O	1.98	0.62
2:B:253:PRO:HD3	2:B:920:ARG:HD3	1.80	0.62
2:B:601:ASN:ND2	2:B:832:GLN:HA	2.13	0.62
2:B:1163:THR:HG21	2:B:1198:TYR:HB2	1.80	0.62
3:E:41:GLN:HA	3:E:41:GLN:NE2	2.12	0.62
3:D:273:MET:HE3	3:D:327:LEU:HB3	1.81	0.62
1:A:429:ILE:HG23	1:A:995:LEU:HD22	1.80	0.62
1:A:907:PHE:O	1:A:911:ILE:HG12	1.99	0.62
2:C:7:LYS:HG2	2:C:978:ASP:OD2	2.00	0.62
2:C:451:PHE:CE2	2:C:1256:VAL:HG22	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:50:ARG:O	3:E:51:GLY:O	2.17	0.62
2:B:822:ILE:HG22	2:B:826:LEU:CD2	2.27	0.62
2:C:1000:GLN:HB3	2:C:1010:ASN:HA	1.82	0.62
1:A:963:MET:HE1	1:A:1118:VAL:HG21	1.81	0.62
1:A:214:HIS:HA	2:B:718:GLN:HE22	1.65	0.62
3:E:31:ARG:H	3:E:41:GLN:HE22	1.46	0.62
1:A:412:LEU:C	1:A:412:LEU:HD23	2.24	0.61
3:E:243:ARG:O	3:E:243:ARG:HG3	1.99	0.61
1:A:307:LEU:HD23	1:A:344:LEU:HD12	1.82	0.61
2:C:744:ASP:O	2:C:812:GLN:HG3	1.99	0.61
3:E:83:ASN:ND2	3:E:85:ARG:HB2	2.15	0.61
1:A:529:VAL:O	1:A:532:PRO:HD2	2.00	0.61
2:C:580:LYS:HE2	2:C:624:GLU:HG2	1.81	0.61
1:A:1073:ILE:HG23	1:A:1074:PRO:HD2	1.81	0.61
2:B:627:TRP:O	2:B:631:ILE:HG12	2.00	0.61
3:E:46:ILE:C	3:E:48:LEU:H	2.08	0.61
1:A:948:ARG:HH21	1:A:957:ASP:HB3	1.64	0.61
2:B:542:LEU:O	2:B:546:ILE:HG22	2.00	0.61
2:C:129:ASN:HD21	2:C:869:THR:H	1.47	0.61
2:C:650:MET:HE2	2:C:678:PHE:CZ	2.35	0.61
2:C:1032:ASN:HD21	2:C:1042:ARG:NH2	1.98	0.61
2:B:451:PHE:O	2:B:452:GLU:HB3	1.99	0.61
2:C:70:GLU:OE2	2:C:911:ASP:OD1	2.17	0.61
2:C:499:PRO:HG3	3:E:45:TRP:CE2	2.36	0.61
2:C:622:SER:HB3	2:C:625:ASN:ND2	2.15	0.61
3:E:328:HIS:HB3	3:E:410:THR:CG2	2.31	0.61
1:A:55:VAL:HG12	1:A:177:ASN:HB2	1.83	0.61
2:C:504:LEU:HG	2:C:506:PRO:HD3	1.81	0.61
3:D:273:MET:HG3	3:D:273:MET:O	2.00	0.61
3:D:350:THR:OG1	3:D:353:GLN:HG3	2.00	0.61
3:E:114:GLN:HB3	3:E:115:PRO:HD2	1.83	0.61
2:C:937:GLN:HE22	2:C:1025:GLN:HE22	1.47	0.61
2:C:1216:SER:HB3	2:C:1217:PRO:HD2	1.81	0.61
2:B:270:PRO:HG3	2:B:297:PRO:HB3	1.83	0.60
2:C:439:MET:HE1	3:E:193:THR:CB	2.27	0.60
2:C:339:LEU:HB3	2:C:353:MET:HE3	1.82	0.60
2:C:603:VAL:HG23	2:C:604:VAL:HG23	1.82	0.60
3:E:158:PHE:HB2	3:E:273:MET:HE3	1.81	0.60
1:A:374:GLN:H	1:A:374:GLN:NE2	2.00	0.60
1:A:446:ARG:HD3	1:A:1071:ALA:O	2.02	0.60
2:C:102:ALA:O	2:C:106:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:THR:HG21	1:A:724:ARG:NH2	2.17	0.60
1:A:456:LEU:HD12	1:A:457:PRO:CD	2.26	0.60
1:A:68:LEU:O	1:A:170:ARG:NH2	2.35	0.60
2:B:321:SER:HA	2:B:368:ASP:OD1	2.02	0.60
2:C:8:THR:HG22	2:C:9:LYS:N	2.17	0.60
2:C:743:ILE:HG22	2:C:744:ASP:N	2.17	0.60
2:B:278:GLN:NE2	2:B:280:VAL:CG2	2.65	0.60
2:C:982:MET:HG2	2:C:983:LEU:N	2.17	0.60
2:C:1147:MET:HE3	2:C:1149:HIS:CE1	2.37	0.60
3:D:117:LEU:HD12	3:D:118:GLN:H	1.67	0.60
1:A:1028:MET:HE2	1:A:1042:LEU:HD22	1.84	0.59
2:B:629:PHE:HB2	2:B:655:MET:HE1	1.84	0.59
2:C:248:LEU:HA	2:C:913:GLU:OE2	2.02	0.59
2:C:763:ASN:C	2:C:763:ASN:HD22	2.09	0.59
2:C:937:GLN:HE22	2:C:1025:GLN:NE2	2.00	0.59
2:B:1095:ARG:NH1	3:E:50:ARG:HB3	2.18	0.59
2:C:2:LYS:HG2	2:C:3:ARG:N	2.15	0.59
3:E:91:PHE:O	3:E:92:LEU:HB2	2.02	0.59
1:A:974:TRP:HB2	1:A:977:CYS:HB3	1.84	0.59
2:B:983:LEU:O	2:B:984:LEU:HB2	2.01	0.59
2:B:1171:THR:HG23	2:B:1172:PRO:CD	2.32	0.59
2:C:580:LYS:HE2	2:C:624:GLU:CG	2.32	0.59
2:C:955:LEU:HD12	2:C:955:LEU:C	2.28	0.59
2:B:502:ASN:HD22	2:B:502:ASN:N	2.00	0.59
3:E:147:LEU:O	3:E:151:THR:HG23	2.02	0.59
1:A:582:VAL:HG21	1:A:591:SER:HB2	1.84	0.59
1:A:646:THR:HG22	1:A:647:ASN:N	2.18	0.59
1:A:22:THR:HG23	1:A:226:LYS:HE3	1.84	0.59
2:B:601:ASN:HD21	2:B:832:GLN:HA	1.66	0.59
1:A:730:LEU:C	1:A:730:LEU:HD23	2.27	0.59
1:A:907:PHE:CZ	1:A:1019:MET:HE1	2.37	0.59
1:A:1028:MET:HE1	1:A:1101:MET:HG3	1.84	0.59
2:B:1131:LYS:HD2	2:B:1160:TRP:CE2	2.38	0.59
1:A:648:ASN:C	1:A:648:ASN:ND2	2.60	0.58
2:C:85:GLY:HA2	2:C:964:THR:HG22	1.85	0.58
2:C:473:ASN:ND2	2:C:474:ILE:H	2.01	0.58
1:A:620:THR:OG1	1:A:623:VAL:HG23	2.03	0.58
2:B:280:VAL:CG2	2:B:281:LEU:H	2.15	0.58
2:C:1079:ARG:HG2	2:C:1079:ARG:NH1	2.16	0.58
2:C:1034:GLU:HG3	2:C:1251:VAL:HG23	1.86	0.58
3:E:22:ASN:C	3:E:22:ASN:ND2	2.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1096:ASP:HB2	2:B:1100:MET:O	2.03	0.58
2:C:242:LYS:O	2:C:242:LYS:HG2	2.04	0.58
1:A:759:SER:HB2	1:A:760:PRO:HD2	1.85	0.58
2:B:533:GLN:HE21	2:B:537:GLN:NE2	2.01	0.58
2:C:931:LEU:O	2:C:935:VAL:HG12	2.04	0.58
3:E:7:LEU:HB3	3:E:125:TYR:O	2.04	0.58
3:E:91:PHE:CZ	3:E:92:LEU:HD12	2.38	0.58
2:C:1112:LEU:HD22	2:C:1141:MET:CE	2.33	0.58
3:E:74:GLY:HA3	3:E:91:PHE:CE2	2.39	0.58
1:A:24:GLN:H	1:A:24:GLN:NE2	2.01	0.58
2:C:528:ASN:HD21	2:C:530:THR:CB	2.15	0.58
3:D:214:GLN:CG	3:D:295:LEU:HD21	2.34	0.58
3:E:406:ASN:O	3:E:410:THR:HG23	2.04	0.58
2:B:610:ASP:CB	2:C:786:THR:HG21	2.32	0.58
2:B:1147:MET:HE3	2:B:1149:HIS:CE1	2.38	0.58
2:C:507:TYR:CE2	2:C:915:PHE:HB3	2.39	0.58
2:C:775:LEU:HD23	2:C:775:LEU:C	2.28	0.58
2:C:776:VAL:HG21	2:C:793:MET:HG2	1.85	0.58
3:E:12:GLY:HA2	3:E:121:ALA:HB1	1.86	0.58
3:E:124:VAL:HG11	3:E:316:ILE:HG23	1.86	0.58
1:A:1129:ALA:HB3	1:A:1144:ASP:HB2	1.85	0.57
2:B:1166:TRP:CD1	2:B:1176:PRO:HG2	2.39	0.57
2:C:400:GLU:CD	2:C:400:GLU:H	2.11	0.57
2:C:837:ARG:HG3	2:C:838:LEU:H	1.68	0.57
2:C:1162:LEU:H	2:C:1162:LEU:HD12	1.69	0.57
2:C:1162:LEU:HD12	2:C:1162:LEU:N	2.19	0.57
2:B:743:ILE:CG2	2:B:744:ASP:N	2.68	0.57
2:C:2:LYS:CG	2:C:3:ARG:H	2.13	0.57
3:D:163:TYR:H	3:D:292:THR:HG21	1.69	0.57
1:A:290:GLN:HE21	1:A:290:GLN:N	2.02	0.57
2:B:332:ILE:HD11	2:B:349:ALA:HB3	1.87	0.57
2:C:1229:VAL:HG13	2:C:1236:THR:HG21	1.86	0.57
1:A:1034:PHE:HA	1:A:1040:CYS:SG	2.45	0.57
2:C:654:ASN:O	2:C:657:VAL:HG23	2.04	0.57
3:E:153:LEU:HG	3:E:153:LEU:O	2.05	0.57
2:C:983:LEU:O	2:C:984:LEU:HB2	2.03	0.57
3:D:50:ARG:HG3	3:D:50:ARG:NH1	2.15	0.57
1:A:54:ILE:HD12	1:A:54:ILE:N	2.19	0.57
2:B:1002:GLN:HG3	2:B:1008:THR:HG22	1.87	0.57
2:C:234:GLN:NE2	2:C:911:ASP:OD1	2.37	0.57
3:D:83:ASN:HD21	3:D:85:ARG:HB2	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:54:THR:HG22	3:E:55:SER:N	2.20	0.57
1:A:836:ILE:HG23	1:A:837:LEU:N	2.20	0.57
2:B:280:VAL:CG2	2:B:281:LEU:N	2.67	0.57
2:B:620:VAL:HG11	2:B:656:MET:SD	2.45	0.57
2:B:851:ARG:HG3	2:B:851:ARG:NH1	2.19	0.57
3:D:130:TYR:CE2	3:D:132:PHE:HB2	2.40	0.57
1:A:221:LEU:HD12	1:A:255:MET:HE3	1.87	0.56
2:B:574:ALA:O	2:B:577:ILE:HG22	2.04	0.56
2:C:1042:ARG:HG2	2:C:1043:GLY:N	2.20	0.56
3:D:246:ASP:HA	3:D:360:LEU:HD21	1.87	0.56
3:E:276:SER:HG	3:E:332:VAL:HG23	1.68	0.56
1:A:854:THR:HG21	1:A:867:PHE:CD2	2.41	0.56
1:A:985:SER:O	1:A:986:TYR:HB3	2.06	0.56
2:C:97:GLU:O	2:C:101:GLU:HG3	2.05	0.56
2:B:772:MET:HE3	2:B:797:LEU:HD21	1.86	0.56
2:B:934:LEU:HD21	2:B:1024:VAL:HG11	1.87	0.56
2:B:983:LEU:H	2:B:985:GLU:HG2	1.70	0.56
2:B:1171:THR:C	2:B:1173:THR:H	2.14	0.56
1:A:1158:ARG:HG3	1:A:1158:ARG:HH11	1.71	0.56
2:B:432:GLY:O	2:B:450:VAL:HG23	2.05	0.56
2:B:455:ASP:OD2	2:B:458:THR:HG23	2.05	0.56
1:A:1216:LEU:HD12	1:A:1216:LEU:H	1.71	0.56
2:B:654:ASN:HD21	2:B:675:ALA:N	2.04	0.56
2:B:1112:LEU:HD13	2:B:1141:MET:HE3	1.88	0.56
2:B:1159:ALA:O	2:B:1163:THR:HG23	2.05	0.56
2:C:205:LEU:HD22	2:C:205:LEU:H	1.70	0.56
3:D:279:TRP:C	3:D:281:MET:H	2.13	0.56
2:C:1032:ASN:O	2:C:1032:ASN:ND2	2.38	0.56
2:C:1175:ILE:HG23	2:C:1175:ILE:O	2.05	0.56
3:E:397:PHE:HB2	3:E:401:GLN:OE1	2.04	0.56
2:C:132:GLU:HA	2:C:867:THR:OG1	2.05	0.56
3:D:64:ARG:O	3:D:68:MET:HG3	2.05	0.56
2:B:1172:PRO:HG2	2:C:53:TYR:CE1	2.41	0.56
2:C:763:ASN:HD21	2:C:767:ARG:HG2	1.69	0.56
2:C:846:MET:O	2:C:1001:TYR:HA	2.05	0.56
1:A:851:ILE:H	1:A:851:ILE:CD1	2.02	0.55
2:C:673:ARG:HH11	2:C:673:ARG:HG2	1.71	0.55
1:A:62:PRO:O	1:A:63:LEU:CB	2.53	0.55
2:B:1229:VAL:HG13	2:B:1236:THR:CG2	2.35	0.55
2:C:129:ASN:ND2	2:C:869:THR:H	2.04	0.55
1:A:1063:PHE:CD1	1:A:1063:PHE:C	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:GLY:CA	2:B:871:VAL:HG13	2.36	0.55
2:B:720:ARG:HG3	2:B:737:GLU:HB3	1.89	0.55
2:C:468:ARG:HB2	2:C:1019:VAL:HG11	1.88	0.55
3:D:203:TRP:CZ3	3:D:213:THR:HG21	2.41	0.55
1:A:631:ILE:C	1:A:633:PRO:HD2	2.31	0.55
2:C:807:THR:N	2:C:808:PRO:HD2	2.21	0.55
2:C:837:ARG:CG	2:C:838:LEU:H	2.19	0.55
3:D:263:ILE:HD13	3:D:418:ILE:HG23	1.88	0.55
1:A:716:PHE:O	1:A:718:ASN:N	2.39	0.55
2:B:518:GLN:HG3	2:B:730:ALA:HB1	1.88	0.55
2:B:537:GLN:O	2:B:540:SER:HB3	2.06	0.55
2:C:59:ILE:O	2:C:63:GLN:HG3	2.06	0.55
1:A:531:GLU:HB3	1:A:532:PRO:HD3	1.86	0.55
2:B:338:LEU:HD11	2:B:968:TRP:CD2	2.42	0.55
2:B:562:THR:HG22	2:B:562:THR:O	2.07	0.55
2:B:691:ILE:HD12	2:B:691:ILE:N	2.12	0.55
2:B:955:LEU:C	2:B:955:LEU:HD12	2.32	0.55
3:D:391:MET:SD	3:D:391:MET:C	2.90	0.55
2:B:871:VAL:HG12	2:B:872:GLY:N	2.20	0.55
2:C:192:SER:HB3	2:C:195:ASP:CB	2.36	0.55
3:E:146:GLN:O	3:E:150:VAL:HG23	2.07	0.55
3:E:305:ASP:OD2	3:E:307:ASN:HB2	2.07	0.55
2:C:1158:ASN:ND2	2:C:1160:TRP:H	2.04	0.55
1:A:60:PHE:O	1:A:64:GLN:HG3	2.06	0.55
2:C:349:ALA:O	2:C:1175:ILE:HG22	2.06	0.55
2:C:1188:HIS:O	2:C:1190:ILE:HG23	2.07	0.55
3:D:83:ASN:ND2	3:D:85:ARG:HB2	2.22	0.55
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.72	0.55
2:B:332:ILE:HG23	2:B:333:HIS:N	2.21	0.55
2:B:367:LEU:HD21	2:B:973:MET:HE3	1.88	0.55
2:B:1266:PRO:HG2	2:B:1269:ALA:HB2	1.89	0.55
2:B:303:ARG:NH1	2:B:1208:SER:HB3	2.22	0.54
3:D:58:VAL:HG11	3:D:64:ARG:HB2	1.89	0.54
3:D:117:LEU:HD12	3:D:118:GLN:N	2.22	0.54
3:E:39:LEU:O	3:E:41:GLN:N	2.40	0.54
1:A:554:VAL:HG22	1:A:555:ALA:N	2.22	0.54
1:A:625:HIS:O	1:A:628:GLU:HB3	2.08	0.54
1:A:1019:MET:HE3	1:A:1021:ILE:HD11	1.89	0.54
2:C:743:ILE:HG22	2:C:744:ASP:O	2.08	0.54
2:C:1000:GLN:HB2	2:C:1009:PHE:O	2.07	0.54
3:D:304:ILE:HD13	3:D:327:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:311:ALA:HA	3:E:314:ARG:NH1	2.22	0.54
2:C:66:THR:HG22	2:C:542:LEU:CD1	2.37	0.54
1:A:841:PRO:HG2	1:A:844:SER:OG	2.07	0.54
2:C:1112:LEU:HG	2:C:1116:GLN:HE21	1.72	0.54
1:A:570:ASP:HB3	1:A:607:ALA:HB2	1.89	0.54
2:B:851:ARG:HH22	2:B:989:SER:CB	2.21	0.54
2:B:1036:ASN:HD22	2:B:1207:ARG:HB3	1.73	0.54
1:A:153:LEU:HD13	1:A:155:GLN:HG3	1.89	0.54
2:B:598:TRP:CH2	2:B:743:ILE:HD12	2.43	0.54
2:C:451:PHE:O	2:C:452:GLU:HB3	2.08	0.54
1:A:1019:MET:HE2	1:A:1021:ILE:HD11	1.89	0.54
2:C:66:THR:HG22	2:C:542:LEU:HD13	1.90	0.54
1:A:209:ARG:HA	1:A:212:TRP:CD1	2.43	0.54
2:C:627:TRP:HA	2:C:627:TRP:CE3	2.42	0.54
1:A:610:GLY:O	1:A:658:VAL:HG23	2.08	0.53
1:A:1013:TYR:CE1	1:A:1017:PRO:HA	2.43	0.53
2:B:386:THR:CG2	2:B:410:ARG:HG3	2.38	0.53
2:B:821:VAL:HG11	2:B:905:ILE:HD13	1.89	0.53
2:B:743:ILE:HG22	2:B:744:ASP:N	2.24	0.53
2:C:852:GLN:HG3	2:C:858:THR:HG21	1.89	0.53
3:D:231:GLN:HE21	3:D:231:GLN:HA	1.72	0.53
1:A:931:ASP:OD1	1:A:932:VAL:N	2.39	0.53
3:D:37:TRP:CZ3	3:D:143:VAL:HG13	2.43	0.53
2:C:10:GLY:HA3	2:C:319:ASP:OD1	2.08	0.53
2:C:474:ILE:CG2	2:C:475:ASN:N	2.70	0.53
2:C:518:GLN:OE1	2:C:829:PRO:HG2	2.08	0.53
3:D:170:MET:HE1	3:D:214:GLN:CB	2.38	0.53
3:E:90:ARG:HG3	3:E:90:ARG:HH11	1.74	0.53
1:A:1216:LEU:HD12	1:A:1216:LEU:N	2.24	0.53
2:B:638:LEU:HD11	2:B:886:LEU:HD21	1.91	0.53
2:B:654:ASN:HD21	2:B:675:ALA:H	1.57	0.53
3:D:276:SER:HG	3:D:332:VAL:HG23	1.71	0.53
3:E:350:THR:HG23	3:E:353:GLN:OE1	2.09	0.53
2:C:339:LEU:HD21	2:C:964:THR:OG1	2.08	0.53
3:D:34:ASN:ND2	3:D:104:LEU:O	2.42	0.53
1:A:733:ASN:HD22	1:A:733:ASN:N	2.06	0.53
3:D:33:GLY:HA3	3:D:41:GLN:NE2	2.23	0.53
1:A:992:ARG:O	1:A:996:LEU:HB2	2.08	0.53
2:B:592:ARG:HG3	2:B:592:ARG:HH11	1.72	0.53
1:A:775:ILE:O	1:A:775:ILE:HD12	2.09	0.53
2:C:264:THR:HB	2:C:454:SER:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:646:VAL:HG21	2:C:684:TRP:CD1	2.43	0.53
2:C:985:GLU:N	2:C:986:PRO:HD2	2.23	0.53
3:E:152:LEU:HD22	3:E:161:ILE:HB	1.91	0.53
2:C:440:MET:HB2	2:C:444:MET:O	2.09	0.53
2:C:749:ASN:OD1	2:C:751:THR:HG23	2.09	0.53
2:C:823:ALA:HB3	2:C:824:PRO:CD	2.39	0.53
3:D:331:GLN:HE21	3:D:334:ARG:H	1.57	0.53
1:A:734:VAL:O	1:A:735:GLY:O	2.27	0.52
2:B:610:ASP:CG	2:C:786:THR:HG21	2.34	0.52
2:C:429:ASN:N	2:C:429:ASN:HD22	2.07	0.52
3:D:246:ASP:OD1	3:D:247:ALA:N	2.42	0.52
2:C:585:ASN:ND2	2:C:880:ARG:HH22	2.07	0.52
2:C:822:ILE:HG22	2:C:826:LEU:HG	1.91	0.52
2:C:941:THR:HG22	2:C:943:TYR:H	1.74	0.52
3:D:336:VAL:O	3:D:339:PHE:HB3	2.09	0.52
1:A:501:THR:HG22	1:A:503:LYS:HB2	1.90	0.52
2:C:817:VAL:O	2:C:821:VAL:HG23	2.08	0.52
1:A:971:ARG:HG3	1:A:971:ARG:HH11	1.75	0.52
2:B:518:GLN:HG2	2:B:521:ARG:HH21	1.74	0.52
2:C:1171:THR:CG2	2:C:1172:PRO:N	2.72	0.52
3:D:328:HIS:HB3	3:D:410:THR:CB	2.39	0.52
1:A:203:THR:OG1	1:A:205:GLU:HG2	2.09	0.52
1:A:227:PRO:O	1:A:229:ASN:N	2.43	0.52
2:C:50:ARG:O	2:C:52:GLN:N	2.42	0.52
2:C:440:MET:HB3	2:C:445:SER:HA	1.91	0.52
2:C:690:ASN:HB3	2:C:693:LEU:CD1	2.40	0.52
3:D:340:CYS:HB3	3:D:354:GLN:HG3	1.91	0.52
3:E:328:HIS:HB3	3:E:410:THR:CB	2.40	0.52
2:B:419:ILE:HG13	2:B:1214:SER:O	2.09	0.52
2:B:985:GLU:N	2:B:986:PRO:CD	2.73	0.52
2:B:619:SER:C	2:B:621:THR:H	2.18	0.52
2:C:675:ALA:C	2:C:677:ALA:H	2.18	0.52
3:D:231:GLN:HA	3:D:231:GLN:NE2	2.25	0.52
1:A:385:GLN:HA	1:A:385:GLN:NE2	2.25	0.52
1:A:456:LEU:HA	1:A:678:PHE:CE2	2.45	0.52
1:A:638:TYR:CD1	1:A:638:TYR:C	2.88	0.52
1:A:934:ARG:HD3	1:A:1208:PHE:O	2.10	0.52
2:B:644:ALA:HB3	2:B:645:PRO:HD3	1.92	0.52
2:C:1158:ASN:HD22	2:C:1159:ALA:N	2.07	0.52
3:E:340:CYS:HB3	3:E:354:GLN:OE1	2.10	0.52
2:C:822:ILE:O	2:C:823:ALA:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:279:TRP:C	3:D:281:MET:N	2.65	0.52
2:B:533:GLN:N	2:B:534:PRO:HD2	2.25	0.51
1:A:1189:ILE:HD12	1:A:1230:LEU:HB2	1.91	0.51
2:B:656:MET:HE3	2:B:660:GLU:HB2	1.92	0.51
2:C:929:GLN:O	2:C:932:VAL:HG22	2.10	0.51
2:B:526:GLY:O	2:B:527:ASN:HB2	2.10	0.51
3:D:7:LEU:HD23	3:D:126:ASP:HB2	1.92	0.51
3:E:233:THR:HG21	3:E:256:SER:HB3	1.92	0.51
2:C:573:PRO:HG3	2:C:792:SER:HB2	1.92	0.51
1:A:775:ILE:HD12	1:A:775:ILE:C	2.35	0.51
2:B:513:GLU:HG2	2:B:1016:PRO:HG3	1.91	0.51
2:B:1193:ALA:HB1	2:B:1194:PRO:HD2	1.93	0.51
2:C:638:LEU:HD11	2:C:886:LEU:HD11	1.93	0.51
2:C:1112:LEU:HD13	2:C:1141:MET:HE3	1.92	0.51
3:D:11:VAL:CG2	3:D:12:GLY:N	2.74	0.51
3:E:391:MET:SD	3:E:391:MET:C	2.93	0.51
1:A:209:ARG:NH2	3:D:202:PRO:O	2.43	0.51
2:B:793:MET:HE3	2:B:797:LEU:HG	1.92	0.51
2:C:70:GLU:OE2	2:C:911:ASP:O	2.29	0.51
2:C:984:LEU:O	2:C:985:GLU:C	2.51	0.51
1:A:186:PRO:HG3	1:A:324:ASN:HD22	1.75	0.51
1:A:422:LEU:HD12	1:A:422:LEU:C	2.36	0.51
1:A:983:PRO:O	1:A:984:LEU:HD12	2.11	0.51
1:A:989:ARG:O	1:A:992:ARG:HG2	2.10	0.51
2:B:527:ASN:O	2:B:873:VAL:HG11	2.10	0.51
2:B:674:ARG:H	2:B:674:ARG:CD	2.24	0.51
3:D:54:THR:CG2	3:D:55:SER:N	2.73	0.51
2:B:526:GLY:HA2	2:B:871:VAL:HG13	1.92	0.51
2:B:807:THR:N	2:B:808:PRO:HD2	2.25	0.51
2:B:775:LEU:HD12	2:B:775:LEU:O	2.10	0.51
2:C:80:THR:O	2:C:88:ARG:HG2	2.11	0.51
2:C:270:PRO:HG3	2:C:297:PRO:HB3	1.93	0.51
2:C:532:ILE:O	2:C:533:GLN:C	2.54	0.51
2:C:619:SER:C	2:C:621:THR:H	2.19	0.51
2:C:1112:LEU:HD22	2:C:1141:MET:HE2	1.92	0.51
1:A:612:PHE:CD1	1:A:612:PHE:C	2.89	0.50
2:B:246:GLN:HE22	2:B:982:MET:H	1.57	0.50
2:B:472:MET:HE2	2:B:506:PRO:HB2	1.92	0.50
2:B:970:ASN:OD1	2:B:984:LEU:HB2	2.12	0.50
2:B:1071:THR:HB	2:B:1074:VAL:HG21	1.92	0.50
2:C:70:GLU:OE2	2:C:913:GLU:OE2	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:309:ARG:HB3	2:C:312:SER:OG	2.12	0.50
2:C:510:SER:OG	2:C:513:GLU:HG3	2.12	0.50
2:C:1141:MET:HE1	2:C:1175:ILE:HD11	1.93	0.50
3:E:158:PHE:HB2	3:E:273:MET:CE	2.41	0.50
2:B:440:MET:HB2	2:B:443:ALA:HB3	1.93	0.50
2:C:97:GLU:HG3	2:C:136:SER:HB2	1.93	0.50
2:C:934:LEU:HD11	2:C:1024:VAL:HG11	1.93	0.50
1:A:505:TYR:CD2	1:A:656:PHE:HB3	2.46	0.50
3:D:306:ASN:ND2	3:D:321:GLY:O	2.44	0.50
2:B:370:LEU:HD22	2:B:465:TRP:CD2	2.47	0.50
2:C:122:TYR:OH	2:C:533:GLN:HA	2.10	0.50
1:A:251:ALA:O	1:A:255:MET:HG3	2.12	0.50
2:B:244:THR:CG2	2:B:534:PRO:HG3	2.41	0.50
2:B:524:ASN:N	2:B:524:ASN:HD22	2.09	0.50
2:C:463:GLY:O	2:C:466:MET:HB3	2.12	0.50
2:B:1171:THR:CG2	2:B:1172:PRO:N	2.74	0.50
2:C:8:THR:HG22	2:C:9:LYS:H	1.76	0.50
2:C:528:ASN:ND2	2:C:530:THR:H	2.09	0.50
3:D:228:ILE:HG23	3:D:232:ASN:O	2.11	0.50
3:D:275:THR:HG23	3:D:330:PHE:H	1.76	0.50
3:E:277:PRO:HD3	3:E:401:GLN:HB3	1.94	0.50
3:E:313:SER:HA	3:E:316:ILE:HD11	1.93	0.50
1:A:54:ILE:HD12	1:A:54:ILE:H	1.77	0.50
1:A:1041:SER:HA	1:A:1089:LEU:O	2.12	0.50
2:B:750:VAL:HG12	2:B:751:THR:N	2.25	0.50
2:B:871:VAL:CG1	2:B:872:GLY:N	2.74	0.50
2:C:158:THR:O	2:C:161:ILE:HG22	2.10	0.50
2:C:216:ILE:C	2:C:218:ARG:N	2.69	0.50
3:E:270:LEU:HD12	3:E:270:LEU:O	2.11	0.50
1:A:484:VAL:HG23	1:A:485:LYS:N	2.26	0.50
2:B:407:TYR:CD2	2:B:431:VAL:HG23	2.46	0.50
2:B:601:ASN:HD22	2:B:602:GLY:N	2.10	0.50
2:B:1188:HIS:O	2:B:1189:ASP:C	2.55	0.50
2:C:1166:TRP:CD1	2:C:1176:PRO:HG2	2.46	0.50
1:A:23:ARG:NH1	1:A:29:ASP:OD1	2.45	0.50
1:A:188:PHE:C	1:A:190:LYS:H	2.20	0.50
1:A:486:ASP:CB	1:A:529:VAL:HG21	2.41	0.50
2:C:394:LEU:HB3	2:C:395:PRO:HD2	1.94	0.50
3:D:92:LEU:O	3:D:93:ARG:HB2	2.11	0.50
3:E:336:VAL:O	3:E:339:PHE:HB3	2.12	0.50
2:B:264:THR:HB	2:B:454:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:241:ASN:C	2:C:243:LYS:H	2.20	0.49
1:A:417:LEU:CD2	1:A:711:ILE:HG13	2.42	0.49
2:C:555:ILE:HG22	2:C:803:ILE:HD11	1.94	0.49
2:C:603:VAL:HG13	2:C:831:PHE:HD2	1.77	0.49
2:C:675:ALA:O	2:C:677:ALA:N	2.45	0.49
2:C:743:ILE:CG2	2:C:744:ASP:N	2.74	0.49
2:C:941:THR:HG22	2:C:943:TYR:N	2.28	0.49
2:C:1034:GLU:OE2	2:C:1231:ARG:NH2	2.45	0.49
1:A:4:VAL:O	1:A:4:VAL:HG23	2.12	0.49
1:A:420:LEU:HD22	1:A:698:ASP:O	2.12	0.49
2:B:428:ARG:NH1	2:B:428:ARG:HG2	2.26	0.49
2:C:805:SER:HB2	2:C:887:LEU:O	2.12	0.49
3:D:46:ILE:HG23	3:D:192:TYR:OH	2.12	0.49
3:D:305:ASP:OD2	3:D:307:ASN:HB2	2.11	0.49
3:E:72:LEU:O	3:E:76:LEU:HB2	2.12	0.49
1:A:2:ALA:O	1:A:3:ASN:HB2	2.11	0.49
1:A:1090:ASP:C	1:A:1091:MET:HG3	2.37	0.49
2:B:490:TYR:CD2	2:B:901:TYR:HB3	2.48	0.49
2:B:524:ASN:C	2:B:525:ILE:HG22	2.36	0.49
2:B:1216:SER:HB3	2:B:1217:PRO:HD2	1.94	0.49
2:C:532:ILE:HD13	2:C:604:VAL:CG2	2.42	0.49
2:C:540:SER:HB2	2:C:592:ARG:CB	2.42	0.49
3:D:227:VAL:HG11	3:D:418:ILE:HD12	1.94	0.49
3:E:179:LEU:CD2	3:E:212:MET:HE3	2.36	0.49
3:E:386:ASN:HD22	3:E:386:ASN:H	1.60	0.49
1:A:489:VAL:HG23	1:A:490:LEU:N	2.27	0.49
1:A:1008:ILE:HD12	1:A:1008:ILE:N	2.27	0.49
2:C:641:ASP:OD2	2:C:641:ASP:C	2.55	0.49
3:E:74:GLY:HA3	3:E:91:PHE:CZ	2.48	0.49
3:E:282:ASP:O	3:E:286:ILE:HG22	2.12	0.49
2:B:1150:TYR:HA	2:B:1182:VAL:O	2.13	0.49
2:C:468:ARG:HD2	2:C:468:ARG:O	2.12	0.49
3:D:33:GLY:HA3	3:D:41:GLN:CD	2.37	0.49
3:D:96:TRP:CZ3	3:D:101:LEU:HB3	2.48	0.49
3:E:29:LEU:O	3:E:31:ARG:N	2.45	0.49
1:A:293:GLY:C	1:A:295:ASP:H	2.20	0.49
1:A:757:ARG:HG3	1:A:757:ARG:HH11	1.77	0.49
1:A:808:THR:HG22	1:A:812:ASN:ND2	2.27	0.49
2:B:674:ARG:HD3	2:B:674:ARG:N	2.26	0.49
2:B:1116:GLN:HB3	2:B:1172:PRO:HA	1.95	0.49
2:C:248:LEU:C	2:C:248:LEU:HD23	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:306:VAL:HG23	2:C:1037:LEU:O	2.13	0.49
2:C:407:TYR:CD2	2:C:431:VAL:HG23	2.48	0.49
2:C:814:LEU:O	2:C:815:ALA:C	2.55	0.49
2:C:1226:HIS:O	2:C:1227:ILE:C	2.55	0.49
3:D:13:PHE:CD2	3:D:121:ALA:HB2	2.47	0.49
3:D:340:CYS:O	3:D:341:ASP:C	2.56	0.49
3:E:6:PHE:HB3	3:E:144:TYR:CE1	2.47	0.49
3:E:11:VAL:CG2	3:E:12:GLY:N	2.75	0.49
3:E:325:ASN:N	3:E:325:ASN:ND2	2.51	0.49
3:E:340:CYS:O	3:E:341:ASP:C	2.55	0.49
1:A:342:THR:HB	1:A:343:PRO:HD2	1.95	0.49
1:A:903:PHE:CZ	1:A:926:VAL:HG13	2.47	0.49
1:A:1135:ASP:OD2	1:A:1137:THR:HG23	2.12	0.49
1:A:1158:ARG:HG3	1:A:1158:ARG:NH1	2.28	0.49
2:B:782:GLN:N	2:B:783:PRO:CD	2.75	0.49
2:B:946:ASP:OD2	3:D:31:ARG:NE	2.38	0.49
2:C:552:ASP:OD1	2:C:554:THR:HG23	2.13	0.49
3:D:7:LEU:CD1	3:D:317:HIS:HB3	2.40	0.49
3:D:55:SER:OG	3:D:56:ALA:N	2.46	0.49
2:B:846:MET:SD	2:B:846:MET:C	2.96	0.49
2:C:560:MET:HE2	2:C:577:ILE:HG21	1.95	0.49
2:C:1074:VAL:HG12	2:C:1075:HIS:N	2.28	0.49
3:D:228:ILE:HD13	3:D:234:TYR:HB2	1.95	0.49
3:E:229:HIS:HD2	3:E:231:GLN:N	1.94	0.49
1:A:51:THR:O	1:A:52:ASN:HB2	2.13	0.49
1:A:640:LEU:HD21	1:A:653:PHE:HD1	1.77	0.49
2:B:244:THR:HG23	2:B:534:PRO:HG3	1.94	0.49
2:B:340:ASN:HD22	2:B:340:ASN:H	1.58	0.49
3:D:360:LEU:C	3:D:360:LEU:CD2	2.86	0.49
2:B:332:ILE:HD11	2:B:349:ALA:CB	2.43	0.48
2:B:391:LEU:N	2:B:391:LEU:CD1	2.76	0.48
2:C:1104:PHE:CD1	2:C:1104:PHE:N	2.81	0.48
1:A:1004:ALA:O	1:A:1008:ILE:HD13	2.12	0.48
2:C:772:MET:O	2:C:776:VAL:HG12	2.12	0.48
3:D:162:SER:HA	3:D:292:THR:HG21	1.95	0.48
2:C:603:VAL:HG13	2:C:831:PHE:CD2	2.49	0.48
2:C:1229:VAL:HG13	2:C:1236:THR:CB	2.43	0.48
3:E:13:PHE:CE2	3:E:121:ALA:HB2	2.49	0.48
3:E:385:ALA:HB3	3:E:386:ASN:ND2	2.28	0.48
1:A:481:ARG:O	1:A:484:VAL:HG22	2.13	0.48
1:A:1016:MET:N	1:A:1017:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:756:ASP:C	2:C:758:THR:H	2.19	0.48
2:B:278:GLN:NE2	2:B:281:LEU:HB2	2.28	0.48
2:B:959:ALA:HB2	2:B:993:ARG:NH2	2.28	0.48
3:D:92:LEU:O	3:D:93:ARG:CB	2.62	0.48
3:D:214:GLN:HG3	3:D:295:LEU:HD21	1.94	0.48
3:D:333:ARG:C	3:D:333:ARG:CD	2.87	0.48
1:A:149:THR:HG22	1:A:150:GLY:N	2.27	0.48
1:A:484:VAL:CG2	1:A:485:LYS:N	2.76	0.48
1:A:507:ARG:O	1:A:510:GLN:HG2	2.12	0.48
1:A:1130:TRP:CD1	1:A:1216:LEU:HD22	2.49	0.48
2:B:855:ASP:OD2	2:C:757:PHE:N	2.47	0.48
2:C:630:PHE:HB2	2:C:772:MET:HE1	1.95	0.48
3:D:330:PHE:HB2	3:D:407:THR:HG23	1.96	0.48
3:E:98:ALA:HB1	3:E:99:PRO:HD2	1.94	0.48
2:C:307:HIS:ND1	2:C:310:TRP:HB3	2.29	0.48
3:D:54:THR:HG22	3:D:55:SER:N	2.28	0.48
3:D:55:SER:HB3	3:D:58:VAL:O	2.13	0.48
3:D:350:THR:HG23	3:D:353:GLN:HE21	1.78	0.48
1:A:720:THR:HG22	1:A:724:ARG:H	1.79	0.48
1:A:1241:LYS:O	1:A:1284:TYR:HA	2.13	0.48
2:B:522:ILE:O	2:B:523:MET:C	2.56	0.48
2:C:203:HIS:HB2	2:C:205:LEU:HD23	1.96	0.48
2:C:850:THR:HG23	2:C:1000:GLN:HE22	1.79	0.48
1:A:49:GLN:NE2	1:A:321:GLN:HG2	2.29	0.48
1:A:1032:GLY:HA3	1:A:1040:CYS:HA	1.96	0.48
1:A:632:LEU:N	1:A:633:PRO:CD	2.74	0.48
2:B:415:ASN:HB3	2:B:417:SER:H	1.78	0.48
2:B:618:GLY:HA2	2:B:625:ASN:OD1	2.14	0.48
2:B:946:ASP:O	2:B:947:ARG:HG3	2.14	0.48
2:C:553:PRO:O	2:C:554:THR:C	2.57	0.48
2:C:1126:PHE:O	2:C:1127:ASP:C	2.57	0.48
1:A:42:PRO:HD2	1:A:43:TRP:CZ3	2.49	0.47
1:A:189:ALA:C	1:A:191:ASP:H	2.22	0.47
1:A:582:VAL:HG13	1:A:587:ASP:CB	2.44	0.47
1:A:809:MET:HE3	1:A:990:TRP:HZ3	1.78	0.47
2:B:432:GLY:C	2:B:450:VAL:HG23	2.39	0.47
1:A:235:LEU:HD23	1:A:236:GLY:N	2.29	0.47
2:B:306:VAL:H	2:B:324:MET:HE2	1.78	0.47
2:B:946:ASP:HB3	2:B:948:TYR:CE1	2.49	0.47
2:C:190:LEU:HD13	2:C:196:LEU:HA	1.96	0.47
2:C:466:MET:HE2	2:C:470:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1032:ASN:HD21	2:C:1042:ARG:HH21	1.62	0.47
2:C:1047:ILE:HA	2:C:1198:TYR:O	2.13	0.47
2:C:1096:ASP:HB2	2:C:1100:MET:O	2.14	0.47
3:D:13:PHE:CE2	3:D:121:ALA:HB2	2.50	0.47
1:A:133:LEU:N	1:A:134:PRO:HD2	2.30	0.47
1:A:647:ASN:OD1	1:A:681:TYR:HA	2.14	0.47
1:A:912:LYS:O	1:A:915:SER:HB2	2.14	0.47
1:A:942:ILE:HG12	1:A:949:TYR:CD2	2.49	0.47
2:B:687:CYS:HA	2:B:693:LEU:HD12	1.96	0.47
2:B:1096:ASP:CG	2:B:1097:GLU:H	2.22	0.47
2:C:695:SER:HB3	2:C:698:ASP:HB2	1.95	0.47
2:C:1067:PHE:CZ	2:C:1107:ASN:HB3	2.49	0.47
3:D:340:CYS:CB	3:D:349:MET:HE1	2.44	0.47
2:B:600:TYR:C	2:B:602:GLY:H	2.23	0.47
2:C:294:SER:HB3	2:C:411:MET:HE1	1.97	0.47
2:C:1241:PRO:HG2	2:C:1244:GLN:HB2	1.95	0.47
3:D:66:TYR:O	3:D:69:SER:HB3	2.14	0.47
1:A:316:ARG:HH11	1:A:333:GLN:NE2	2.12	0.47
1:A:680:ARG:HG3	1:A:680:ARG:HH11	1.80	0.47
1:A:840:ILE:O	1:A:840:ILE:HD12	2.14	0.47
1:A:986:TYR:CD1	1:A:1058:ASN:HB3	2.50	0.47
2:B:402:TRP:O	2:B:406:MET:HB2	2.15	0.47
2:B:475:ASN:HB2	2:B:476:PRO:HD2	1.97	0.47
2:B:814:LEU:HD23	2:B:891:TYR:OH	2.15	0.47
2:B:929:GLN:HG2	3:D:32:ALA:O	2.14	0.47
2:B:982:MET:CB	2:B:985:GLU:HG3	2.43	0.47
2:C:350:ASN:HA	2:C:1173:THR:O	2.15	0.47
2:C:943:TYR:CD1	2:C:944:PRO:HD2	2.48	0.47
2:C:1171:THR:C	2:C:1173:THR:N	2.73	0.47
3:D:153:LEU:HD13	3:D:160:PRO:HG3	1.96	0.47
3:E:29:LEU:HD11	3:E:67:GLN:HB3	1.95	0.47
1:A:3:ASN:C	1:A:3:ASN:HD22	2.22	0.47
1:A:646:THR:CG2	1:A:647:ASN:N	2.76	0.47
1:A:721:GLN:O	1:A:722:ALA:C	2.58	0.47
2:C:673:ARG:HG2	2:C:673:ARG:NH1	2.29	0.47
2:C:790:VAL:O	2:C:794:ARG:HG3	2.15	0.47
3:D:38:GLN:O	3:D:39:LEU:C	2.58	0.47
3:D:227:VAL:CG1	3:D:418:ILE:HD12	2.45	0.47
2:B:309:ARG:HB3	2:B:312:SER:HB2	1.96	0.47
2:B:422:PHE:O	2:B:423:VAL:C	2.58	0.47
2:B:490:TYR:CD2	2:B:901:TYR:CB	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:931:LEU:O	2:B:935:VAL:HG23	2.15	0.47
2:C:87:THR:HG21	2:C:140:ASP:HA	1.96	0.47
2:C:532:ILE:HD13	2:C:604:VAL:HG22	1.96	0.47
2:C:1104:PHE:N	2:C:1104:PHE:HD1	2.13	0.47
3:D:231:GLN:HE21	3:D:231:GLN:CA	2.28	0.47
3:D:328:HIS:HB3	3:D:410:THR:CG2	2.44	0.47
1:A:583:ASP:OD2	1:A:583:ASP:N	2.39	0.47
1:A:1250:LEU:O	1:A:1251:ASN:HB2	2.14	0.47
2:B:673:ARG:HE	2:B:674:ARG:NH2	2.12	0.47
2:C:65:ALA:HB2	2:C:545:ARG:HD2	1.96	0.47
2:C:419:ILE:O	2:C:422:PHE:HB3	2.15	0.47
3:D:13:PHE:HE1	3:D:19:VAL:HG22	1.80	0.47
1:A:641:ILE:HG22	1:A:642:LYS:N	2.30	0.46
2:C:475:ASN:OD1	2:C:477:THR:HB	2.15	0.46
3:E:273:MET:O	3:E:273:MET:HG3	2.15	0.46
1:A:203:THR:HG23	1:A:206:VAL:CG2	2.44	0.46
2:B:428:ARG:HG2	2:B:428:ARG:HH11	1.79	0.46
2:B:581:LEU:O	2:B:582:ARG:C	2.57	0.46
2:B:601:ASN:HD21	2:B:832:GLN:CA	2.28	0.46
2:C:757:PHE:N	2:C:757:PHE:CD1	2.82	0.46
3:E:333:ARG:CD	3:E:333:ARG:C	2.88	0.46
1:A:512:VAL:HG12	1:A:513:ALA:N	2.30	0.46
1:A:1225:ASN:C	1:A:1281:PRO:HB3	2.41	0.46
2:B:627:TRP:CH2	2:B:793:MET:HE1	2.50	0.46
2:C:474:ILE:HG22	2:C:475:ASN:N	2.30	0.46
3:E:263:ILE:CD1	3:E:418:ILE:HG23	2.43	0.46
1:A:719:MET:HA	1:A:719:MET:CE	2.40	0.46
2:B:817:VAL:O	2:B:818:GLU:C	2.58	0.46
2:B:1138:ARG:NH2	2:B:1202:THR:HG21	2.30	0.46
2:C:94:GLU:HG3	2:C:134:SER:O	2.16	0.46
2:C:355:ARG:HB3	2:C:954:SER:HB2	1.97	0.46
2:C:540:SER:HB2	2:C:592:ARG:HB3	1.98	0.46
2:C:962:ALA:O	2:C:965:PHE:HB3	2.14	0.46
3:D:279:TRP:O	3:D:281:MET:N	2.48	0.46
1:A:115:VAL:O	1:A:116:ALA:C	2.59	0.46
1:A:188:PHE:HA	1:A:241:MET:SD	2.55	0.46
1:A:203:THR:HG23	1:A:206:VAL:HG23	1.98	0.46
1:A:713:ASN:ND2	1:A:750:ARG:H	2.13	0.46
1:A:930:THR:CG2	1:A:1017:PRO:HG3	2.46	0.46
2:B:268:ILE:HG22	2:B:297:PRO:HG2	1.98	0.46
2:C:181:TYR:OH	2:C:193:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:437:ALA:HB2	2:C:447:TRP:CD1	2.50	0.46
2:B:281:LEU:HD13	2:B:281:LEU:HA	1.76	0.46
2:B:386:THR:HG22	2:B:410:ARG:HG3	1.98	0.46
2:B:704:GLN:O	2:B:708:ILE:HG13	2.15	0.46
2:C:122:TYR:CD2	2:C:875:LEU:HD13	2.50	0.46
2:C:344:LEU:HD12	2:C:1171:THR:CG2	2.46	0.46
2:C:630:PHE:CZ	2:C:634:LEU:HD22	2.50	0.46
2:C:660:GLU:OE2	2:C:701:ILE:HB	2.16	0.46
3:E:90:ARG:HG3	3:E:90:ARG:NH1	2.31	0.46
1:A:64:GLN:H	1:A:117:ASN:ND2	2.13	0.46
1:A:396:TRP:CH2	1:A:398:PRO:HB3	2.51	0.46
1:A:446:ARG:NH1	1:A:1070:ALA:C	2.74	0.46
2:B:601:ASN:HD22	2:B:601:ASN:C	2.22	0.46
2:B:601:ASN:HA	2:B:604:VAL:O	2.16	0.46
2:B:673:ARG:O	2:B:674:ARG:C	2.58	0.46
2:B:1009:PHE:CD1	2:B:1009:PHE:N	2.83	0.46
2:B:1166:TRP:CZ3	2:B:1170:ILE:HD11	2.51	0.46
3:D:170:MET:HE1	3:D:214:GLN:HB3	1.96	0.46
1:A:64:GLN:O	1:A:169:GLY:HA3	2.16	0.46
2:B:660:GLU:OE2	2:B:702:LEU:HB2	2.16	0.46
2:B:945:VAL:HG22	2:B:946:ASP:N	2.30	0.46
2:C:609:ASP:OD1	2:C:610:ASP:OD2	2.33	0.46
2:C:833:VAL:HG13	2:C:834:PRO:HD2	1.98	0.46
3:D:229:HIS:CD2	3:D:231:GLN:H	2.34	0.46
3:E:213:THR:HB	3:E:291:LEU:HD21	1.97	0.46
1:A:24:GLN:CD	1:A:24:GLN:N	2.64	0.46
1:A:564:ARG:HB3	1:A:565:PRO:HD2	1.97	0.46
2:B:520:ILE:O	2:B:523:MET:HB2	2.16	0.46
2:B:990:GLY:HA3	2:C:804:LYS:HB2	1.97	0.46
2:C:1171:THR:C	2:C:1173:THR:H	2.21	0.46
3:D:126:ASP:OD1	3:D:126:ASP:C	2.59	0.46
1:A:1012:MET:HE2	1:A:1016:MET:HE1	1.97	0.46
1:A:1036:VAL:CG2	1:A:1122:PRO:HD3	2.46	0.46
2:B:519:ILE:O	2:B:520:ILE:C	2.59	0.46
2:B:923:ILE:O	2:B:924:THR:C	2.59	0.46
2:B:1119:THR:HG22	2:B:1120:ARG:N	2.28	0.46
2:C:413:THR:N	2:C:414:PRO:CD	2.72	0.46
2:C:660:GLU:HG2	2:C:699:ALA:HA	1.96	0.46
1:A:340:ASN:HB3	1:A:345:TRP:CH2	2.50	0.45
1:A:577:ASP:OD1	1:A:577:ASP:O	2.34	0.45
1:A:823:ASP:O	1:A:844:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:468:ARG:HB2	2:C:1019:VAL:CG1	2.45	0.45
2:C:627:TRP:HA	2:C:627:TRP:HE3	1.81	0.45
2:C:732:LEU:HD13	2:C:999:ILE:HG21	1.97	0.45
3:E:186:THR:HG22	3:E:252:ILE:HG12	1.99	0.45
3:E:329:GLY:O	3:E:410:THR:HG21	2.16	0.45
2:B:654:ASN:ND2	2:B:675:ALA:H	2.14	0.45
2:B:691:ILE:H	2:B:691:ILE:CD1	2.03	0.45
2:B:1088:ASN:HB2	3:E:40:THR:HG21	1.98	0.45
2:C:422:PHE:O	2:C:425:SER:N	2.47	0.45
3:D:228:ILE:HG23	3:D:233:THR:HA	1.98	0.45
3:D:263:ILE:CD1	3:D:418:ILE:HG23	2.47	0.45
3:E:9:LYS:H	3:E:151:THR:CG2	2.28	0.45
2:B:411:MET:HG2	2:B:412:GLY:N	2.31	0.45
2:C:77:ASP:O	2:C:78:GLU:C	2.59	0.45
2:C:507:TYR:CD2	2:C:915:PHE:HB3	2.51	0.45
2:B:397:PRO:O	2:B:398:ASP:HB3	2.17	0.45
2:B:566:SER:HB3	2:B:569:GLN:HG2	1.99	0.45
2:B:600:TYR:C	2:B:602:GLY:N	2.75	0.45
2:B:824:PRO:HB2	2:B:825:MET:HE2	1.98	0.45
2:C:981:ASP:HB3	2:C:982:MET:H	1.62	0.45
2:C:1034:GLU:CD	2:C:1231:ARG:HH21	2.25	0.45
2:C:1061:PRO:HA	2:C:1062:PRO:HD3	1.71	0.45
2:C:1150:TYR:CZ	2:C:1182:VAL:HG21	2.52	0.45
3:E:107:ALA:HA	3:E:108:PRO:HD3	1.86	0.45
1:A:250:ASN:O	1:A:251:ALA:C	2.59	0.45
1:A:525:ASP:O	1:A:555:ALA:HB3	2.16	0.45
1:A:582:VAL:CG2	1:A:591:SER:HB2	2.46	0.45
2:B:521:ARG:O	2:B:524:ASN:ND2	2.49	0.45
2:B:906:TYR:N	2:B:907:PRO:HD2	2.32	0.45
2:B:958:SER:C	2:B:960:ALA:N	2.74	0.45
1:A:938:GLY:O	1:A:952:PRO:HG2	2.16	0.45
2:B:671:GLN:O	2:B:671:GLN:HG2	2.17	0.45
2:B:991:ASP:OD2	2:B:991:ASP:C	2.59	0.45
2:C:63:GLN:O	2:C:64:ARG:C	2.60	0.45
2:C:325:ALA:HB1	2:C:326:PRO:HD2	1.98	0.45
2:C:1162:LEU:H	2:C:1162:LEU:CD1	2.30	0.45
3:E:109:PRO:HG2	3:E:110:GLN:NE2	2.31	0.45
3:E:270:LEU:C	3:E:270:LEU:CD1	2.88	0.45
1:A:533:TRP:NE1	1:A:544:PRO:HD3	2.32	0.45
2:B:526:GLY:HA3	2:B:871:VAL:HG13	1.98	0.45
2:C:772:MET:HE3	2:C:797:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:291:LEU:C	3:D:293:GLY:N	2.72	0.45
3:E:60:THR:HG22	3:E:281:MET:HE3	1.97	0.45
1:A:1145:ILE:HD11	1:A:1183:MET:HB2	1.99	0.45
2:C:906:TYR:HB3	2:C:907:PRO:CD	2.47	0.45
3:D:42:PHE:O	3:D:46:ILE:HG22	2.17	0.45
3:E:98:ALA:HB1	3:E:99:PRO:CD	2.46	0.45
3:E:333:ARG:O	3:E:333:ARG:HD3	2.17	0.45
3:E:369:ARG:HG3	3:E:402:TRP:CZ2	2.52	0.45
1:A:421:PRO:O	1:A:422:LEU:HB3	2.16	0.45
1:A:515:PHE:N	1:A:575:TYR:O	2.50	0.45
1:A:668:SER:O	1:A:671:TYR:HB3	2.17	0.45
1:A:716:PHE:O	1:A:717:SER:C	2.60	0.45
2:B:588:PHE:O	2:B:589:SER:C	2.59	0.45
2:B:601:ASN:ND2	2:B:601:ASN:C	2.74	0.45
2:C:94:GLU:CB	2:C:133:LEU:HD22	2.42	0.45
2:C:150:MET:O	2:C:154:ILE:HG13	2.17	0.45
2:C:782:GLN:HG3	2:C:785:TRP:CE3	2.51	0.45
3:D:7:LEU:HA	3:D:125:TYR:O	2.16	0.45
1:A:185:PRO:HA	1:A:186:PRO:HD3	1.82	0.45
1:A:402:ILE:C	1:A:402:ILE:HD12	2.42	0.45
1:A:554:VAL:HG22	1:A:555:ALA:H	1.80	0.45
1:A:743:ILE:N	1:A:743:ILE:HD12	2.31	0.45
1:A:1028:MET:CE	1:A:1042:LEU:HD13	2.47	0.45
2:B:372:LEU:HD23	2:B:372:LEU:HA	1.81	0.45
2:B:473:ASN:HD21	2:B:504:LEU:HA	1.80	0.45
3:D:10:THR:HB	3:D:73:SER:HB3	1.99	0.45
3:D:357:ILE:O	3:D:358:GLU:C	2.60	0.45
1:A:712:GLU:O	1:A:713:ASN:C	2.61	0.44
1:A:721:GLN:C	1:A:725:ILE:HG12	2.41	0.44
2:B:619:SER:C	2:B:621:THR:N	2.76	0.44
2:C:534:PRO:O	2:C:535:VAL:C	2.58	0.44
3:E:41:GLN:HB3	3:E:68:MET:HE2	1.98	0.44
3:E:117:LEU:HD12	3:E:118:GLN:N	2.32	0.44
3:E:165:ARG:CZ	3:E:170:MET:HE3	2.48	0.44
3:E:241:CYS:HB2	3:E:251:TRP:CE3	2.51	0.44
2:B:313:ASN:C	2:B:313:ASN:ND2	2.73	0.44
2:B:527:ASN:CA	2:B:873:VAL:HG13	2.40	0.44
2:B:670:THR:HG23	2:B:672:SER:H	1.82	0.44
2:C:192:SER:HB3	2:C:195:ASP:CG	2.42	0.44
2:C:757:PHE:N	2:C:757:PHE:HD1	2.16	0.44
3:E:263:ILE:CD1	3:E:418:ILE:HD12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TYR:CD2	1:A:232:HIS:HB3	2.51	0.44
2:B:681:PRO:C	2:B:683:THR:N	2.76	0.44
2:B:807:THR:HG21	2:B:886:LEU:HD23	1.99	0.44
2:C:190:LEU:HD11	2:C:199:HIS:CD2	2.52	0.44
2:C:1131:LYS:HG2	2:C:1132:THR:HG23	1.99	0.44
3:D:226:GLY:C	3:D:342:ARG:HD2	2.42	0.44
3:D:359:ALA:O	3:D:362:ASP:HB2	2.18	0.44
3:E:130:TYR:CE2	3:E:132:PHE:HB2	2.52	0.44
3:E:206:ASP:O	3:E:211:ARG:NH1	2.50	0.44
1:A:329:SER:O	1:A:332:SER:HB3	2.17	0.44
1:A:460:TYR:O	1:A:469:ARG:NH2	2.48	0.44
2:B:547:SER:HA	2:B:818:GLU:OE2	2.17	0.44
2:B:572:SER:O	2:B:573:PRO:C	2.60	0.44
2:B:1017:GLY:HA3	3:D:41:GLN:HG2	1.98	0.44
2:B:1065:LEU:HD23	2:B:1065:LEU:HA	1.84	0.44
3:D:75:THR:HG21	3:D:104:LEU:HD11	1.99	0.44
3:D:182:TYR:HE1	3:D:212:MET:HE1	1.82	0.44
3:D:228:ILE:HG22	3:D:229:HIS:N	2.31	0.44
3:E:76:LEU:HD11	3:E:147:LEU:HD21	1.99	0.44
3:E:85:ARG:HH21	3:E:87:GLY:H	1.65	0.44
3:E:241:CYS:HB2	3:E:251:TRP:CD2	2.53	0.44
3:E:303:LEU:HD13	3:E:321:GLY:HA3	1.99	0.44
3:E:333:ARG:HH22	3:E:358:GLU:HB3	1.82	0.44
1:A:872:TYR:HA	1:A:877:TRP:CZ2	2.53	0.44
2:B:602:GLY:HA3	2:B:831:PHE:CD2	2.52	0.44
2:C:135:ARG:HD3	2:C:989:SER:HB2	1.99	0.44
3:D:7:LEU:HD23	3:D:126:ASP:HA	2.00	0.44
3:D:62:GLY:HA3	3:D:280:ASN:HA	1.98	0.44
3:D:150:VAL:HG12	3:D:154:ASN:ND2	2.32	0.44
3:D:383:ASN:ND2	3:D:390:THR:HA	2.32	0.44
3:E:340:CYS:SG	3:E:349:MET:HE1	2.57	0.44
2:B:340:ASN:N	2:B:340:ASN:ND2	2.53	0.44
2:B:814:LEU:O	2:B:815:ALA:C	2.60	0.44
2:B:955:LEU:HD12	2:B:955:LEU:O	2.17	0.44
2:C:378:PHE:N	2:C:378:PHE:CD1	2.86	0.44
2:C:499:PRO:HG3	3:E:45:TRP:CD2	2.53	0.44
2:C:821:VAL:HG12	2:C:821:VAL:O	2.17	0.44
2:C:1032:ASN:ND2	2:C:1042:ARG:HH21	2.15	0.44
2:C:1163:THR:HG22	2:C:1199:ILE:HD12	2.00	0.44
1:A:671:TYR:O	1:A:675:VAL:HG23	2.17	0.44
1:A:1052:VAL:HG12	1:A:1053:PHE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:VAL:HG23	2:B:1235:LEU:O	2.18	0.44
2:B:673:ARG:HE	2:B:674:ARG:NH1	2.15	0.44
2:B:681:PRO:C	2:B:683:THR:H	2.26	0.44
2:B:702:LEU:HD12	2:B:702:LEU:HA	1.74	0.44
2:C:511:ASN:O	2:C:515:GLN:HG3	2.18	0.44
2:C:738:VAL:HG12	2:C:739:LEU:N	2.33	0.44
2:C:1163:THR:HG21	2:C:1198:TYR:HB2	1.99	0.44
3:E:99:PRO:C	3:E:101:LEU:H	2.26	0.44
1:A:632:LEU:HD22	1:A:638:TYR:CD2	2.53	0.44
1:A:685:SER:O	1:A:689:ARG:HB2	2.17	0.44
2:B:1096:ASP:CB	2:B:1100:MET:O	2.64	0.44
2:C:74:LYS:NZ	2:C:530:THR:HG21	2.33	0.44
2:C:619:SER:C	2:C:621:THR:N	2.76	0.44
2:C:923:ILE:O	2:C:924:THR:C	2.60	0.44
2:C:941:THR:HG22	2:C:942:GLN:N	2.31	0.44
3:E:377:ARG:O	3:E:378:GLU:C	2.61	0.44
1:A:666:TRP:HA	1:A:666:TRP:CE3	2.53	0.44
1:A:922:VAL:HG12	1:A:924:VAL:HG23	1.99	0.44
1:A:923:LEU:HD12	1:A:923:LEU:N	2.33	0.44
1:A:934:ARG:HD2	1:A:1209:TYR:HA	2.00	0.44
2:C:44:GLU:HG3	2:C:45:PRO:HD2	2.00	0.44
3:E:350:THR:OG1	3:E:353:GLN:HG3	2.18	0.44
1:A:43:TRP:HB2	1:A:57:VAL:CG1	2.47	0.43
1:A:274:GLN:HA	1:A:275:PRO:HD3	1.80	0.43
1:A:907:PHE:CZ	1:A:911:ILE:HD11	2.53	0.43
2:C:344:LEU:HD12	2:C:1171:THR:HG21	2.00	0.43
2:C:782:GLN:HE21	2:C:782:GLN:HB3	1.67	0.43
2:C:925:CYS:O	2:C:926:GLU:C	2.60	0.43
1:A:19:GLU:OE2	1:A:225:ASP:OD1	2.36	0.43
1:A:249:ILE:HG23	1:A:253:ASP:HB2	2.00	0.43
2:C:1081:CYS:HB2	2:C:1094:ILE:HD11	2.00	0.43
3:D:48:LEU:O	3:D:49:GLY:C	2.60	0.43
1:A:735:GLY:O	1:A:736:ASN:HB2	2.18	0.43
1:A:869:GLU:O	1:A:870:LEU:HB3	2.19	0.43
1:A:1035:ILE:HG22	1:A:1036:VAL:N	2.33	0.43
2:B:636:LEU:N	2:B:637:PRO:HD2	2.32	0.43
2:B:641:ASP:OD2	2:B:641:ASP:C	2.60	0.43
2:B:1097:GLU:O	2:B:1097:GLU:HG2	2.16	0.43
2:B:1159:ALA:HB2	2:B:1181:MET:SD	2.57	0.43
2:C:44:GLU:HA	2:C:45:PRO:HD3	1.76	0.43
2:C:216:ILE:C	2:C:218:ARG:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:378:PHE:CE2	2:C:433:ARG:HB2	2.53	0.43
3:D:78:ILE:HB	3:D:79:PRO:CD	2.48	0.43
2:B:852:GLN:OE1	2:C:804:LYS:NZ	2.50	0.43
2:C:518:GLN:HE21	2:C:518:GLN:HB3	1.57	0.43
2:C:824:PRO:HB2	2:C:825:MET:HE2	2.00	0.43
2:C:963:ALA:HA	2:C:992:PRO:HG3	1.99	0.43
1:A:401:THR:HG21	1:A:724:ARG:HH21	1.81	0.43
1:A:459:THR:O	1:A:465:GLU:HG3	2.19	0.43
1:A:757:ARG:HG3	1:A:757:ARG:NH1	2.33	0.43
1:A:1195:LEU:HG	1:A:1197:TYR:CE1	2.52	0.43
2:B:244:THR:HG23	2:B:534:PRO:CG	2.48	0.43
2:B:391:LEU:N	2:B:391:LEU:HD12	2.34	0.43
2:B:645:PRO:HG3	2:B:713:TRP:CE2	2.54	0.43
2:C:146:ASN:HA	2:C:153:ARG:HH21	1.83	0.43
2:C:1111:PRO:HG2	2:C:1114:LEU:HG	1.99	0.43
1:A:155:GLN:HA	2:B:746:GLN:HE21	1.84	0.43
1:A:270:ALA:O	1:A:271:ARG:NH1	2.51	0.43
1:A:1073:ILE:HG22	1:A:1074:PRO:N	2.33	0.43
1:A:1073:ILE:CG2	1:A:1074:PRO:HD2	2.47	0.43
2:B:261:GLY:O	2:B:1259:ARG:NH2	2.50	0.43
2:B:736:PRO:O	2:B:737:GLU:HB2	2.18	0.43
2:C:935:VAL:HG13	2:C:936:ALA:N	2.33	0.43
3:D:130:TYR:HE2	3:D:132:PHE:HB2	1.82	0.43
1:A:873:LEU:HD23	1:A:873:LEU:HA	1.89	0.43
1:A:1242:GLU:CB	1:A:1247:ILE:HD11	2.48	0.43
2:B:823:ALA:CA	2:B:826:LEU:HD23	2.40	0.43
2:B:991:ASP:HA	2:B:992:PRO:HD3	1.68	0.43
2:C:76:ASN:C	2:C:76:ASN:HD22	2.27	0.43
2:C:973:MET:HE2	2:C:973:MET:HB3	1.87	0.43
2:C:1119:THR:HG22	2:C:1120:ARG:N	2.34	0.43
2:C:1152:ASP:HA	2:C:1153:PRO:HD3	1.80	0.43
3:D:7:LEU:CD2	3:D:126:ASP:HB2	2.48	0.43
3:D:273:MET:HE3	3:D:327:LEU:CB	2.48	0.43
1:A:772:LEU:HD12	1:A:773:PRO:HD2	2.00	0.43
1:A:924:VAL:O	1:A:926:VAL:HG23	2.18	0.43
1:A:976:ASN:HA	1:A:1027:PRO:HG2	2.00	0.43
1:A:982:VAL:HG23	1:A:1018:ILE:O	2.18	0.43
2:B:946:ASP:HB2	2:B:1025:GLN:OE1	2.19	0.43
2:C:439:MET:HE2	2:C:439:MET:HB3	1.92	0.43
2:C:619:SER:O	2:C:621:THR:N	2.52	0.43
3:D:275:THR:HG23	3:D:330:PHE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:66:TYR:O	3:E:69:SER:HB3	2.18	0.43
1:A:316:ARG:HA	1:A:317:PRO:HD3	1.82	0.43
1:A:582:VAL:CG1	1:A:587:ASP:HB2	2.47	0.43
2:B:619:SER:O	2:B:621:THR:N	2.51	0.43
2:C:241:ASN:OD1	2:C:243:LYS:HB2	2.19	0.43
2:C:1118:ASN:O	2:C:1119:THR:C	2.62	0.43
3:D:145:GLN:HG2	3:D:294:CYS:HA	2.01	0.43
3:E:176:ASN:C	3:E:176:ASN:ND2	2.68	0.43
3:E:404:ARG:O	3:E:405:GLY:C	2.62	0.43
2:B:518:GLN:HE22	2:B:828:PHE:HE1	1.62	0.43
2:B:664:MET:HG3	2:B:671:GLN:N	2.33	0.43
2:B:1171:THR:C	2:B:1173:THR:N	2.75	0.43
2:C:473:ASN:ND2	2:C:474:ILE:N	2.66	0.43
2:C:765:ARG:HG3	2:C:765:ARG:NH1	2.33	0.43
2:C:806:MET:O	2:C:809:MET:HB3	2.18	0.43
2:C:846:MET:HE3	2:C:846:MET:HB2	1.85	0.43
2:C:1068:ASP:O	2:C:1071:THR:HB	2.19	0.43
3:D:144:TYR:O	3:D:145:GLN:C	2.62	0.43
3:D:273:MET:HE1	3:D:327:LEU:HD13	1.96	0.43
2:B:829:PRO:HA	2:B:830:PRO:HD3	1.89	0.42
2:B:947:ARG:HG2	2:B:947:ARG:HH11	1.84	0.42
2:B:1048:GLY:O	2:B:1198:TYR:HA	2.20	0.42
2:C:591:PHE:O	2:C:594:ALA:HB3	2.19	0.42
2:C:969:VAL:O	2:C:973:MET:HG3	2.19	0.42
2:C:1019:VAL:HG23	2:C:1020:ILE:H	1.83	0.42
2:C:1052:SER:OG	2:C:1053:THR:N	2.52	0.42
3:E:8:PHE:CA	3:E:151:THR:HG21	2.46	0.42
1:A:709:ILE:HG12	1:A:730:LEU:HD12	2.00	0.42
1:A:940:LEU:HD22	1:A:1016:MET:HE2	2.00	0.42
1:A:947:LYS:O	1:A:959:PRO:HA	2.19	0.42
2:C:360:HIS:O	2:C:363:LEU:HB3	2.19	0.42
3:D:78:ILE:HB	3:D:79:PRO:HD3	2.01	0.42
3:E:85:ARG:NH2	3:E:87:GLY:H	2.17	0.42
3:E:92:LEU:O	3:E:93:ARG:HB2	2.19	0.42
1:A:67:VAL:HG12	1:A:169:GLY:HA2	2.01	0.42
1:A:458:ASP:OD2	1:A:458:ASP:N	2.52	0.42
2:C:1058:PRO:HD2	2:C:1182:VAL:HG12	2.02	0.42
3:D:7:LEU:HD23	3:D:126:ASP:CB	2.49	0.42
3:D:12:GLY:HA2	3:D:121:ALA:HB1	2.01	0.42
3:D:273:MET:O	3:D:329:GLY:HA2	2.19	0.42
3:D:369:ARG:O	3:D:370:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:46:ILE:C	3:E:48:LEU:N	2.77	0.42
3:E:81:ARG:NH2	3:E:88:ASP:OD1	2.50	0.42
1:A:293:GLY:O	1:A:295:ASP:N	2.52	0.42
1:A:330:PHE:CE2	1:A:334:ILE:HD11	2.54	0.42
1:A:1015:TYR:CD1	1:A:1015:TYR:N	2.87	0.42
1:A:1183:MET:HE1	1:A:1214:LEU:HD13	2.02	0.42
2:B:525:ILE:O	2:B:526:GLY:C	2.63	0.42
2:B:1096:ASP:HB3	2:B:1100:MET:N	2.23	0.42
2:B:1139:ILE:HG22	2:B:1141:MET:HG2	2.01	0.42
2:B:1160:TRP:O	2:B:1161:ASN:C	2.62	0.42
2:C:40:PRO:O	2:C:41:ALA:C	2.63	0.42
2:C:76:ASN:HB3	2:C:524:ASN:ND2	2.35	0.42
2:C:511:ASN:O	2:C:512:ALA:C	2.62	0.42
3:D:63:SER:HB3	3:D:393:ARG:O	2.19	0.42
3:E:158:PHE:CD2	3:E:275:THR:HB	2.54	0.42
1:A:1033:ASN:O	1:A:1035:ILE:N	2.52	0.42
1:A:1036:VAL:HG23	1:A:1120:ASP:O	2.19	0.42
1:A:1237:GLU:HA	1:A:1250:LEU:O	2.19	0.42
2:B:415:ASN:HD22	2:B:415:ASN:HA	1.50	0.42
2:B:473:ASN:ND2	2:B:504:LEU:HA	2.34	0.42
2:C:239:VAL:HG22	2:C:240:GLU:H	1.83	0.42
2:C:335:PHE:CE2	2:C:1040:ILE:HD11	2.54	0.42
2:C:664:MET:HE2	2:C:670:THR:O	2.19	0.42
2:C:1111:PRO:O	2:C:1112:LEU:C	2.63	0.42
3:E:153:LEU:O	3:E:395:LYS:NZ	2.52	0.42
1:A:494:TYR:HD2	1:A:542:PRO:HD2	1.79	0.42
1:A:934:ARG:CD	1:A:1209:TYR:HA	2.49	0.42
2:B:332:ILE:CG2	2:B:333:HIS:N	2.82	0.42
2:B:347:ARG:HG2	2:B:347:ARG:HH11	1.85	0.42
2:B:708:ILE:O	2:B:709:ILE:C	2.61	0.42
2:C:761:LEU:HD23	2:C:761:LEU:HA	1.88	0.42
3:E:234:TYR:CE2	3:E:235:ARG:HD2	2.55	0.42
1:A:263:GLN:HE22	1:A:267:ASN:ND2	2.17	0.42
1:A:471:LEU:HD21	1:A:691:LEU:HB2	2.01	0.42
1:A:480:ASP:OD2	1:A:528:LEU:HD12	2.19	0.42
1:A:501:THR:CG2	1:A:503:LYS:HB2	2.49	0.42
1:A:743:ILE:HA	1:A:751:VAL:O	2.20	0.42
2:B:523:MET:HG2	2:B:849:VAL:HG21	2.02	0.42
2:B:635:ALA:O	2:B:636:LEU:C	2.62	0.42
2:B:681:PRO:O	2:B:683:THR:N	2.52	0.42
2:B:1226:HIS:O	2:B:1227:ILE:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:338:LEU:HB3	2:C:339:LEU:H	1.54	0.42
2:C:407:TYR:HD2	2:C:431:VAL:HG23	1.84	0.42
2:C:581:LEU:O	2:C:880:ARG:HD2	2.20	0.42
2:C:828:PHE:HA	2:C:829:PRO:HD2	1.86	0.42
2:C:1131:LYS:HD2	2:C:1160:TRP:CE2	2.55	0.42
1:A:472:PHE:HD2	1:A:646:THR:HG23	1.85	0.42
1:A:486:ASP:HB2	1:A:529:VAL:HG21	2.01	0.42
1:A:499:PRO:C	1:A:501:THR:H	2.27	0.42
1:A:718:ASN:HB3	1:A:719:MET:H	1.57	0.42
1:A:1101:MET:HB3	1:A:1114:LEU:HD12	2.01	0.42
2:B:347:ARG:HG2	2:B:347:ARG:NH1	2.35	0.42
2:B:920:ARG:O	2:B:921:ASP:C	2.62	0.42
2:B:1082:ARG:HA	2:C:1272:MET:HE1	2.02	0.42
2:B:1173:THR:O	2:B:1173:THR:HG22	2.18	0.42
2:B:1182:VAL:HG23	2:B:1183:PRO:HD2	2.00	0.42
2:B:1229:VAL:HG13	2:B:1236:THR:CB	2.50	0.42
2:C:91:LEU:N	2:C:91:LEU:HD12	2.35	0.42
2:C:473:ASN:HD22	2:C:474:ILE:N	2.16	0.42
2:C:600:TYR:HE2	2:C:828:PHE:O	2.03	0.42
2:C:672:SER:O	2:C:673:ARG:C	2.63	0.42
2:C:1018:SER:HB3	2:C:1021:ALA:HB3	2.02	0.42
3:E:13:PHE:CE1	3:E:19:VAL:N	2.88	0.42
1:A:1199:ARG:HA	1:A:1210:ILE:O	2.20	0.42
1:A:1199:ARG:HB3	1:A:1207:GLY:CA	2.50	0.42
2:B:601:ASN:HD21	2:B:833:VAL:H	1.66	0.42
2:B:880:ARG:HG2	2:B:880:ARG:HH11	1.84	0.42
2:C:541:VAL:O	2:C:542:LEU:C	2.62	0.42
3:D:72:LEU:O	3:D:76:LEU:HB2	2.20	0.42
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.81	0.42
1:A:625:HIS:CE1	1:A:629:GLN:HG3	2.55	0.42
2:B:529:ALA:C	2:B:531:VAL:H	2.28	0.42
2:B:754:THR:O	2:B:755:LEU:C	2.61	0.42
2:C:281:LEU:O	2:C:282:ALA:HB2	2.19	0.42
2:C:643:CYS:O	2:C:644:ALA:C	2.63	0.42
2:C:721:TYR:CD1	2:C:721:TYR:C	2.98	0.42
2:C:1185:SER:OG	2:C:1223:PRO:HG2	2.19	0.42
3:D:47:SER:O	3:D:49:GLY:N	2.53	0.42
3:E:144:TYR:O	3:E:145:GLN:C	2.63	0.42
3:E:398:THR:O	3:E:401:GLN:HB2	2.20	0.42
1:A:684:LEU:HD23	1:A:684:LEU:HA	1.85	0.41
1:A:1112:VAL:O	1:A:1112:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:932:VAL:CG2	2:B:933:THR:N	2.81	0.41
2:C:673:ARG:O	2:C:674:ARG:C	2.62	0.41
3:D:50:ARG:NH1	3:D:50:ARG:CG	2.80	0.41
3:D:166:VAL:HG21	3:D:417:LEU:HB3	2.02	0.41
3:D:172:SER:OG	3:D:175:VAL:HG23	2.20	0.41
1:A:293:GLY:C	1:A:295:ASP:N	2.78	0.41
1:A:494:TYR:CE1	1:A:506:LEU:HD13	2.54	0.41
1:A:548:ARG:HG3	1:A:548:ARG:HH11	1.85	0.41
1:A:833:GLU:H	1:A:833:GLU:CD	2.28	0.41
1:A:856:GLN:HA	1:A:857:PRO:HD3	1.85	0.41
2:B:870:THR:HG22	2:B:871:VAL:N	2.35	0.41
2:B:981:ASP:HB2	2:B:982:MET:H	1.68	0.41
2:C:932:VAL:HG23	2:C:933:THR:N	2.35	0.41
2:C:1171:THR:CG2	2:C:1172:PRO:CD	2.96	0.41
3:D:7:LEU:HD23	3:D:126:ASP:CA	2.49	0.41
3:E:23:ASP:O	3:E:24:GLU:C	2.63	0.41
3:E:47:SER:C	3:E:48:LEU:HG	2.44	0.41
1:A:3:ASN:ND2	1:A:7:VAL:O	2.53	0.41
1:A:60:PHE:O	1:A:62:PRO:O	2.38	0.41
2:C:343:THR:HG22	2:C:1173:THR:CG2	2.50	0.41
2:C:675:ALA:C	2:C:677:ALA:N	2.76	0.41
2:C:983:LEU:H	2:C:985:GLU:HG2	1.86	0.41
3:E:41:GLN:HE21	3:E:41:GLN:CA	2.10	0.41
1:A:207:LEU:O	1:A:210:PHE:HB3	2.20	0.41
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.80	0.41
1:A:446:ARG:NH1	1:A:1070:ALA:HA	2.35	0.41
1:A:1058:ASN:C	1:A:1060:ALA:H	2.27	0.41
2:B:394:LEU:HD12	2:B:402:TRP:CG	2.54	0.41
2:B:1175:ILE:O	2:B:1175:ILE:HG13	2.17	0.41
2:C:1255:ASN:OD1	2:C:1255:ASN:N	2.53	0.41
3:E:167:ASP:HB2	3:E:267:ASN:OD1	2.20	0.41
3:E:235:ARG:O	3:E:236:THR:OG1	2.35	0.41
3:E:322:ARG:HH11	3:E:322:ARG:HG2	1.85	0.41
1:A:357:SER:HA	1:A:358:PRO:HD3	1.91	0.41
1:A:928:CYS:HA	1:A:929:PRO:HD3	1.88	0.41
2:B:805:SER:HB2	2:B:887:LEU:O	2.21	0.41
2:B:1217:PRO:O	2:B:1218:GLN:HB3	2.21	0.41
2:C:616:ASP:HA	2:C:674:ARG:HH21	1.86	0.41
2:C:665:ASP:HB3	2:C:686:ARG:HD3	2.02	0.41
2:C:822:ILE:C	2:C:824:PRO:HD2	2.46	0.41
2:C:955:LEU:C	2:C:955:LEU:CD1	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLY:O	1:A:149:THR:O	2.39	0.41
1:A:377:LEU:O	1:A:379:MET:N	2.53	0.41
2:B:268:ILE:N	2:B:268:ILE:HD12	2.36	0.41
2:B:684:TRP:HE3	2:B:689:MET:HE3	1.86	0.41
2:B:958:SER:O	2:B:960:ALA:N	2.54	0.41
2:C:70:GLU:CD	2:C:911:ASP:OD1	2.64	0.41
2:C:145:SER:C	2:C:147:GLN:H	2.29	0.41
2:C:161:ILE:HD12	2:C:161:ILE:HA	1.76	0.41
2:C:1061:PRO:HG3	2:C:1201:SER:O	2.21	0.41
2:C:1213:ASN:ND2	2:C:1219:THR:OG1	2.42	0.41
3:D:47:SER:C	3:D:49:GLY:N	2.78	0.41
3:D:152:LEU:HD22	3:D:161:ILE:HB	2.02	0.41
3:D:193:THR:O	3:D:194:LEU:C	2.64	0.41
3:E:114:GLN:CB	3:E:115:PRO:HD2	2.45	0.41
3:E:369:ARG:O	3:E:370:ASP:C	2.61	0.41
1:A:112:ASN:O	1:A:113:VAL:C	2.64	0.41
1:A:680:ARG:O	1:A:681:TYR:C	2.63	0.41
2:B:627:TRP:CE3	2:B:627:TRP:HA	2.55	0.41
2:B:638:LEU:HD23	2:B:638:LEU:HA	1.88	0.41
2:B:685:PRO:HG2	2:B:688:PHE:HB2	2.03	0.41
2:B:1102:VAL:HA	2:B:1103:PRO:HD3	1.86	0.41
2:B:1111:PRO:O	2:B:1112:LEU:C	2.64	0.41
2:C:543:LEU:HA	2:C:546:ILE:HG22	2.03	0.41
2:C:1034:GLU:HG3	2:C:1251:VAL:CG2	2.49	0.41
3:D:333:ARG:C	3:D:333:ARG:HD2	2.46	0.41
3:E:275:THR:HG23	3:E:330:PHE:H	1.86	0.41
1:A:1036:VAL:HG21	1:A:1122:PRO:HD3	2.02	0.41
2:B:880:ARG:HG2	2:B:880:ARG:NH1	2.36	0.41
2:B:1063:PRO:O	2:B:1065:LEU:N	2.54	0.41
2:B:1111:PRO:HA	2:B:1140:GLU:HB2	2.03	0.41
2:C:919:GLN:O	2:C:922:MET:HB3	2.21	0.41
3:D:86:TRP:CZ3	3:D:98:ALA:HA	2.56	0.41
3:D:165:ARG:HD3	3:D:214:GLN:NE2	2.36	0.41
3:E:77:GLN:HG2	3:E:125:TYR:OH	2.20	0.41
3:E:133:LEU:HD23	3:E:139:PHE:CD2	2.56	0.41
3:E:241:CYS:HB2	3:E:251:TRP:CZ3	2.56	0.41
1:A:825:VAL:HG12	1:A:826:LEU:N	2.36	0.41
1:A:940:LEU:HD22	1:A:1016:MET:CE	2.50	0.41
2:B:499:PRO:HB3	3:D:183:PHE:CE2	2.56	0.41
2:B:502:ASN:N	2:B:502:ASN:ND2	2.68	0.41
2:B:1158:ASN:OD1	2:B:1158:ASN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:691:ILE:H	2:C:691:ILE:CD1	2.09	0.41
2:C:929:GLN:HG2	2:C:1018:SER:HB2	2.03	0.41
2:C:941:THR:CG2	2:C:942:GLN:N	2.83	0.41
2:C:1150:TYR:CD2	2:C:1182:VAL:HG23	2.55	0.41
2:C:1241:PRO:HA	2:C:1242:PRO:HD3	1.86	0.41
3:D:98:ALA:HB1	3:D:99:PRO:CD	2.50	0.41
3:D:225:VAL:O	3:D:225:VAL:HG12	2.20	0.41
3:E:279:TRP:C	3:E:281:MET:N	2.78	0.41
1:A:922:VAL:C	1:A:923:LEU:HD12	2.46	0.41
1:A:951:PHE:HA	1:A:952:PRO:HD2	1.92	0.41
2:B:483:LEU:HA	2:B:483:LEU:HD23	1.84	0.41
2:B:926:GLU:OE2	2:B:1018:SER:HA	2.21	0.41
2:B:958:SER:C	2:B:960:ALA:H	2.29	0.41
2:C:44:GLU:HG3	2:C:45:PRO:CD	2.51	0.41
2:C:81:PRO:HA	2:C:87:THR:HA	2.02	0.41
2:C:900:TRP:CD1	2:C:900:TRP:C	2.99	0.41
2:C:1158:ASN:C	2:C:1158:ASN:ND2	2.69	0.41
3:D:37:TRP:CZ3	3:D:143:VAL:CG1	3.04	0.41
3:E:92:LEU:O	3:E:93:ARG:CB	2.69	0.41
3:E:95:VAL:HG23	3:E:107:ALA:HB2	2.02	0.41
3:E:273:MET:O	3:E:329:GLY:HA2	2.21	0.41
1:A:3:ASN:O	1:A:341:GLU:HB2	2.20	0.40
1:A:66:LEU:HD22	1:A:73:TYR:CE2	2.56	0.40
1:A:976:ASN:HA	1:A:1027:PRO:CG	2.50	0.40
2:B:601:ASN:HD22	2:B:601:ASN:N	2.18	0.40
2:B:840:ARG:O	2:B:841:ASP:C	2.63	0.40
2:B:1019:VAL:HG23	2:B:1020:ILE:N	2.36	0.40
2:B:1152:ASP:OD1	2:B:1152:ASP:C	2.64	0.40
2:C:840:ARG:O	2:C:841:ASP:C	2.65	0.40
1:A:350:TYR:C	1:A:350:TYR:CD1	2.99	0.40
1:A:750:ARG:NH1	1:A:750:ARG:CG	2.72	0.40
1:A:1029:GLU:HB3	1:A:1043:VAL:HB	2.03	0.40
2:B:919:GLN:O	2:B:922:MET:HB3	2.21	0.40
2:B:1173:THR:O	2:B:1173:THR:CG2	2.69	0.40
2:B:1219:THR:HB	2:B:1224:ASP:OD1	2.22	0.40
2:C:218:ARG:HH22	2:C:241:ASN:HB3	1.86	0.40
2:C:528:ASN:ND2	2:C:530:THR:N	2.69	0.40
3:E:216:ILE:O	3:E:217:LEU:C	2.65	0.40
3:E:306:ASN:CB	3:E:314:ARG:HD3	2.36	0.40
1:A:836:ILE:CG2	1:A:837:LEU:N	2.84	0.40
2:B:497:TYR:O	2:B:498:ALA:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:822:ILE:O	2:B:823:ALA:C	2.64	0.40
2:B:1190:ILE:C	2:B:1191:SER:O	2.64	0.40
2:C:759:ASN:OD1	2:C:759:ASN:C	2.64	0.40
2:C:776:VAL:O	2:C:776:VAL:HG22	2.21	0.40
2:C:863:SER:HB2	2:C:865:SER:OG	2.21	0.40
2:C:1044:ASP:OD1	2:C:1140:GLU:HA	2.22	0.40
3:D:270:LEU:C	3:D:270:LEU:CD1	2.88	0.40
3:D:277:PRO:C	3:D:279:TRP:H	2.30	0.40
3:D:406:ASN:O	3:D:407:THR:C	2.64	0.40
1:A:21:ARG:HG2	1:A:21:ARG:HH11	1.87	0.40
1:A:223:HIS:O	1:A:227:PRO:HG3	2.21	0.40
1:A:772:LEU:HA	1:A:773:PRO:HD2	1.97	0.40
1:A:938:GLY:O	1:A:953:LYS:HE2	2.21	0.40
1:A:978:SER:HB2	1:A:1025:GLY:HA3	2.03	0.40
2:B:306:VAL:HG23	2:B:1037:LEU:O	2.20	0.40
2:B:691:ILE:N	2:B:691:ILE:CD1	2.80	0.40
2:B:778:ASN:O	2:B:780:ARG:N	2.54	0.40
2:C:410:ARG:HH11	2:C:410:ARG:HG2	1.87	0.40
2:C:605:THR:CG2	2:C:870:THR:HG21	2.46	0.40
2:C:873:VAL:HA	2:C:874:PRO:HD3	1.78	0.40
3:D:276:SER:OG	3:D:278:ASP:OD1	2.38	0.40
3:D:377:ARG:O	3:D:378:GLU:C	2.64	0.40
3:E:19:VAL:HA	3:E:20:PRO:HD3	1.80	0.40
3:E:39:LEU:C	3:E:41:GLN:N	2.69	0.40
3:E:264:ARG:HA	3:E:265:PRO:HD3	1.96	0.40
3:E:279:TRP:C	3:E:281:MET:H	2.29	0.40
1:A:1135:ASP:O	1:A:1141:THR:HG22	2.22	0.40
2:C:469:LEU:HD23	2:C:469:LEU:HA	1.88	0.40
2:C:695:SER:C	2:C:697:ILE:H	2.30	0.40
2:C:968:TRP:C	2:C:970:ASN:N	2.74	0.40
3:E:189:GLU:O	3:E:193:THR:HG23	2.22	0.40
3:E:312:VAL:HG23	3:E:313:SER:N	2.37	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	1280/1289 (99%)	1131 (88%)	125 (10%)	24 (2%)	6	33
2	B	1027/1275 (80%)	872 (85%)	135 (13%)	20 (2%)	6	33
2	C	1211/1275 (95%)	1063 (88%)	127 (10%)	21 (2%)	7	35
3	D	415/418 (99%)	359 (86%)	46 (11%)	10 (2%)	4	29
3	E	415/418 (99%)	361 (87%)	41 (10%)	13 (3%)	3	25
All	All	4348/4675 (93%)	3786 (87%)	474 (11%)	88 (2%)	6	32

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	THR
1	A	193	SER
1	A	717	SER
1	A	735	GLY
1	A	945	THR
1	A	947	LYS
1	A	986	TYR
2	B	855	ASP
2	C	51	GLU
2	C	983	LEU
3	D	317	HIS
3	E	48	LEU
3	E	51	GLY
3	E	317	HIS
3	E	322	ARG
3	E	405	GLY
1	A	38	PRO
1	A	228	THR
1	A	520	GLY
1	A	719	MET
1	A	877	TRP
1	A	1034	PHE
2	B	319	ASP
2	B	589	SER
2	B	779	GLN
2	B	1214	SER
2	C	3	ARG

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Mol	Chain	Res	Type
2	C	676	SER
3	D	48	LEU
3	D	404	ARG
3	D	405	GLY
3	E	40	THR
3	E	312	VAL
1	A	119	LEU
1	A	152	SER
1	A	294	GLU
1	A	1202	GLN
2	B	502	ASN
2	B	1254	TYR
2	C	78	GLU
2	C	412	GLY
2	C	837	ARG
2	C	1096	ASP
2	C	1214	SER
3	D	128	ASP
3	E	30	LEU
1	A	225	ASP
1	A	349	ARG
1	A	721	GLN
2	B	525	ILE
2	B	530	THR
2	B	620	VAL
2	B	1191	SER
2	C	338	LEU
2	C	620	VAL
2	C	823	ALA
2	C	1254	TYR
3	E	52	LEU
3	E	128	ASP
1	A	3	ASN
1	A	801	ALA
2	B	523	MET
2	B	1063	PRO
2	C	200	VAL
2	C	1127	ASP
3	D	20	PRO
2	B	452	GLU
2	B	893	PRO
2	B	1054	HIS

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Mol	Chain	Res	Type
2	B	1064	ASP
2	B	1228	PRO
2	C	327	PRO
2	C	533	GLN
2	C	714	PRO
2	C	1228	PRO
3	D	131	PRO
3	D	278	ASP
3	D	280	ASN
3	E	311	ALA
1	A	530	ILE
2	B	637	PRO
3	D	46	ILE
1	A	876	GLY
2	B	753	PRO
2	C	1175	ILE
3	E	20	PRO
3	E	131	PRO
2	C	834	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1118/1121 (100%)	1066 (95%)	52 (5%)	23	50
2	B	911/1115 (82%)	853 (94%)	58 (6%)	16	43
2	C	1070/1115 (96%)	1013 (95%)	57 (5%)	20	48
3	D	352/353 (100%)	333 (95%)	19 (5%)	20	47
3	E	352/353 (100%)	337 (96%)	15 (4%)	26	52
All	All	3803/4057 (94%)	3602 (95%)	201 (5%)	20	48

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	38	PRO
1	A	111	VAL
1	A	117	ASN
1	A	119	LEU
1	A	170	ARG
1	A	203	THR
1	A	205	GLU
1	A	223	HIS
1	A	263	GLN
1	A	281	GLN
1	A	290	GLN
1	A	294	GLU
1	A	295	ASP
1	A	332	SER
1	A	350	TYR
1	A	361	VAL
1	A	374	GLN
1	A	377	LEU
1	A	385	GLN
1	A	413	MET
1	A	436	SER
1	A	455	GLN
1	A	490	LEU
1	A	529	VAL
1	A	583	ASP
1	A	591	SER
1	A	648	ASN
1	A	654	VAL
1	A	663	SER
1	A	693	SER
1	A	719	MET
1	A	750	ARG
1	A	755	THR
1	A	779	SER
1	A	804	HIS
1	A	851	ILE
1	A	908	GLN
1	A	928	CYS
1	A	946	ASN
1	A	957	ASP
1	A	980	THR
1	A	982	VAL

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Mol	Chain	Res	Type
1	A	998	SER
1	A	1026	LEU
1	A	1091	MET
1	A	1123	ASP
1	A	1138	ILE
1	A	1141	THR
1	A	1155	THR
1	A	1265	THR
1	A	1268	ILE
2	B	242	LYS
2	B	249	HIS
2	B	251	ASP
2	B	254	ARG
2	B	256	VAL
2	B	281	LEU
2	B	302	SER
2	B	313	ASN
2	B	337	GLN
2	B	338	LEU
2	B	340	ASN
2	B	341	THR
2	B	353	MET
2	B	386	THR
2	B	406	MET
2	B	415	ASN
2	B	444	MET
2	B	455	ASP
2	B	492	THR
2	B	518	GLN
2	B	524	ASN
2	B	525	ILE
2	B	546	ILE
2	B	601	ASN
2	B	615	LYS
2	B	686	ARG
2	B	692	GLN
2	B	702	LEU
2	B	739	LEU
2	B	750	VAL
2	B	767	ARG
2	B	770	GLU
2	B	772	MET

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Mol	Chain	Res	Type
2	B	814	LEU
2	B	833	VAL
2	B	836	VAL
2	B	851	ARG
2	B	852	GLN
2	B	911	ASP
2	B	932	VAL
2	B	939	SER
2	B	942	GLN
2	B	961	THR
2	B	973	MET
2	B	985	GLU
2	B	1027	THR
2	B	1064	ASP
2	B	1066	VAL
2	B	1080	ASP
2	B	1081	CYS
2	B	1085	PHE
2	B	1093	MET
2	B	1163	THR
2	B	1171	THR
2	B	1182	VAL
2	B	1206	ASP
2	B	1230	GLU
2	B	1243	THR
2	C	42	THR
2	C	56	ARG
2	C	73	MET
2	C	129	ASN
2	C	147	GLN
2	C	206	HIS
2	C	216	ILE
2	C	217	GLN
2	C	221	THR
2	C	252	THR
2	C	254	ARG
2	C	302	SER
2	C	338	LEU
2	C	400	GLU
2	C	409	THR
2	C	410	ARG
2	C	411	MET

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Mol	Chain	Res	Type
2	C	429	ASN
2	C	455	ASP
2	C	473	ASN
2	C	501	VAL
2	C	503	ARG
2	C	518	GLN
2	C	528	ASN
2	C	601	ASN
2	C	615	LYS
2	C	665	ASP
2	C	680	THR
2	C	689	MET
2	C	750	VAL
2	C	751	THR
2	C	763	ASN
2	C	765	ARG
2	C	772	MET
2	C	777	ASP
2	C	782	GLN
2	C	785	TRP
2	C	792	SER
2	C	814	LEU
2	C	863	SER
2	C	887	LEU
2	C	934	LEU
2	C	985	GLU
2	C	995	THR
2	C	1019	VAL
2	C	1027	THR
2	C	1064	ASP
2	C	1066	VAL
2	C	1071	THR
2	C	1119	THR
2	C	1171	THR
2	C	1175	ILE
2	C	1206	ASP
2	C	1230	GLU
2	C	1248	PRO
2	C	1255	ASN
2	C	1268	THR
3	D	10	THR
3	D	34	ASN

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Mol	Chain	Res	Type
3	D	50	ARG
3	D	92	LEU
3	D	100	THR
3	D	101	LEU
3	D	202	PRO
3	D	206	ASP
3	D	213	THR
3	D	255	CYS
3	D	258	ASN
3	D	295	LEU
3	D	312	VAL
3	D	346	ASP
3	D	366	GLN
3	D	391	MET
3	D	394	THR
3	D	398	THR
3	D	410	THR
3	E	7	LEU
3	E	22	ASN
3	E	41	GLN
3	E	43	LEU
3	E	44	ASP
3	E	48	LEU
3	E	50	ARG
3	E	105	VAL
3	E	176	ASN
3	E	204	GLU
3	E	325	ASN
3	E	360	LEU
3	E	386	ASN
3	E	391	MET
3	E	394	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (158) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	37	ASN
1	A	52	ASN
1	A	58	GLN
1	A	71	GLN
1	A	117	ASN

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Mol	Chain	Res	Type
1	A	139	ASN
1	A	155	GLN
1	A	158	GLN
1	A	180	ASN
1	A	263	GLN
1	A	267	ASN
1	A	281	GLN
1	A	290	GLN
1	A	333	GLN
1	A	347	GLN
1	A	352	GLN
1	A	373	ASN
1	A	374	GLN
1	A	385	GLN
1	A	404	GLN
1	A	428	ASN
1	A	466	GLN
1	A	492	HIS
1	A	510	GLN
1	A	526	GLN
1	A	535	GLN
1	A	625	HIS
1	A	648	ASN
1	A	660	GLN
1	A	713	ASN
1	A	733	ASN
1	A	812	ASN
1	A	862	ASN
1	A	1038	GLN
1	A	1079	GLN
1	A	1110	ASN
1	A	1211	GLN
1	A	1251	ASN
1	A	1253	GLN
2	B	241	ASN
2	B	246	GLN
2	B	278	GLN
2	B	293	GLN
2	B	313	ASN
2	B	375	HIS
2	B	382	HIS
2	B	415	ASN

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Mol	Chain	Res	Type
2	B	421	ASN
2	B	502	ASN
2	B	524	ASN
2	B	533	GLN
2	B	537	GLN
2	B	544	GLN
2	B	569	GLN
2	B	601	ASN
2	B	654	ASN
2	B	692	GLN
2	B	704	GLN
2	B	710	HIS
2	B	715	ASN
2	B	745	HIS
2	B	746	GLN
2	B	778	ASN
2	B	782	GLN
2	B	996	GLN
2	B	1032	ASN
2	B	1036	ASN
2	B	1051	GLN
2	B	1107	ASN
2	B	1116	GLN
2	B	1125	GLN
2	B	1149	HIS
2	B	1188	HIS
2	B	1233	ASN
2	B	1246	GLN
2	C	76	ASN
2	C	93	ASN
2	C	129	ASN
2	C	138	ASN
2	C	141	ASN
2	C	147	GLN
2	C	199	HIS
2	C	208	ASN
2	C	229	ASN
2	C	234	GLN
2	C	246	GLN
2	C	375	HIS
2	C	380	GLN
2	C	382	HIS

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Mol	Chain	Res	Type
2	C	390	ASN
2	C	429	ASN
2	C	438	GLN
2	C	473	ASN
2	C	518	GLN
2	C	524	ASN
2	C	528	ASN
2	C	585	ASN
2	C	601	ASN
2	C	625	ASN
2	C	654	ASN
2	C	671	GLN
2	C	682	HIS
2	C	704	GLN
2	C	710	HIS
2	C	763	ASN
2	C	774	ASN
2	C	779	GLN
2	C	782	GLN
2	C	937	GLN
2	C	1000	GLN
2	C	1002	GLN
2	C	1025	GLN
2	C	1032	ASN
2	C	1033	HIS
2	C	1107	ASN
2	C	1116	GLN
2	C	1125	GLN
2	C	1149	HIS
2	C	1158	ASN
2	C	1233	ASN
2	C	1244	GLN
3	D	17	GLN
3	D	34	ASN
3	D	41	GLN
3	D	114	GLN
3	D	141	HIS
3	D	146	GLN
3	D	205	HIS
3	D	214	GLN
3	D	229	HIS
3	D	231	GLN

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Mol	Chain	Res	Type
3	D	258	ASN
3	D	267	ASN
3	D	331	GLN
3	D	351	GLN
3	D	353	GLN
3	D	354	GLN
3	D	383	ASN
3	E	22	ASN
3	E	38	GLN
3	E	41	GLN
3	E	110	GLN
3	E	141	HIS
3	E	146	GLN
3	E	154	ASN
3	E	176	ASN
3	E	181	ASN
3	E	185	HIS
3	E	200	ASN
3	E	229	HIS
3	E	242	ASN
3	E	315	ASN
3	E	325	ASN
3	E	365	GLN
3	E	383	ASN
3	E	386	ASN
3	E	399	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.