



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:03 PM UTC

PDB ID : 1FNW / pdb_00001fnw
Title : CRYSTAL STRUCTURE OF STREPTOCOCCAL PYROGENIC EXO-TOXIN A
Authors : Earhart, C.A.; Vath, G.M.; Roggiani, M.; Schlivert, P.M.; Ohlendorf, D.H.
Deposited on : 2000-08-23
Resolution : 3.90 Å(reported)

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

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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

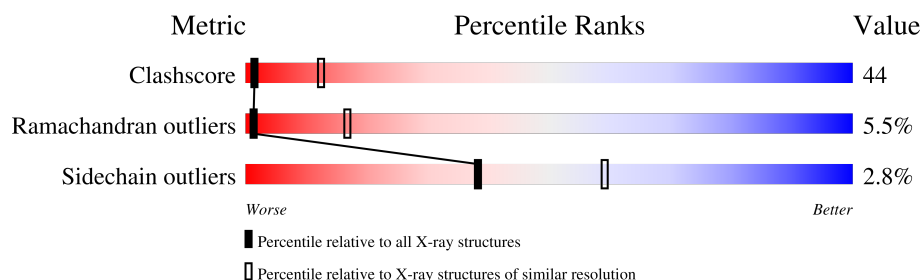
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)

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	221	37% 49% 14%
1	B	221	40% 50% 10%
1	C	221	38% 53% 9%
1	D	221	37% 53% 10%
1	E	221	39% 53% 7%
1	F	221	38% 55% 7%
1	G	221	37% 54% 8%
1	H	221	39% 52% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14616 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 EXOTOXIN TYPE A PRECURSOR (ALLELE 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	B	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	C	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	D	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	E	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	F	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	G	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	H	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	THR	LEU	conflict	UNP P62560
A	154	ILE	THR	conflict	UNP P62560
A	209	ASN	SER	conflict	UNP P62560
A	210	LYS	ASN	conflict	UNP P62560
B	453	THR	LEU	conflict	UNP P62560
B	454	ILE	THR	conflict	UNP P62560
B	509	ASN	SER	conflict	UNP P62560
B	510	LYS	ASN	conflict	UNP P62560
C	753	THR	LEU	conflict	UNP P62560
C	754	ILE	THR	conflict	UNP P62560
C	809	ASN	SER	conflict	UNP P62560
C	810	LYS	ASN	conflict	UNP P62560
D	1053	THR	LEU	conflict	UNP P62560

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1054	ILE	THR	conflict	UNP P62560
D	1109	ASN	SER	conflict	UNP P62560
D	1110	LYS	ASN	conflict	UNP P62560
E	1353	THR	LEU	conflict	UNP P62560
E	1354	ILE	THR	conflict	UNP P62560
E	1409	ASN	SER	conflict	UNP P62560
E	1410	LYS	ASN	conflict	UNP P62560
F	1653	THR	LEU	conflict	UNP P62560
F	1654	ILE	THR	conflict	UNP P62560
F	1709	ASN	SER	conflict	UNP P62560
F	1710	LYS	ASN	conflict	UNP P62560
G	1953	THR	LEU	conflict	UNP P62560
G	1954	ILE	THR	conflict	UNP P62560
G	2009	ASN	SER	conflict	UNP P62560
G	2010	LYS	ASN	conflict	UNP P62560
H	2253	THR	LEU	conflict	UNP P62560
H	2254	ILE	THR	conflict	UNP P62560
H	2309	ASN	SER	conflict	UNP P62560
H	2310	LYS	ASN	conflict	UNP P62560

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

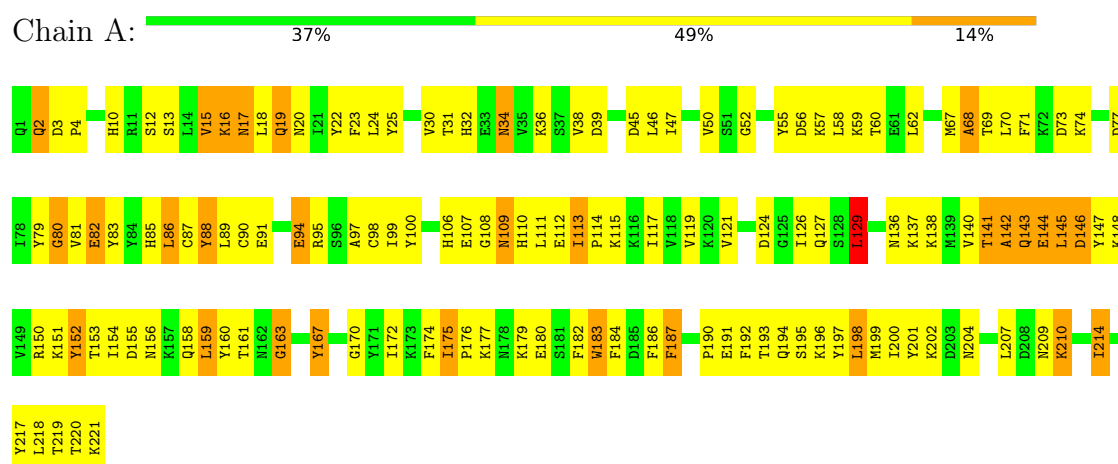
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Cd 4 4	0	0
2	B	4	Total Cd 4 4	0	0
2	C	4	Total Cd 4 4	0	0
2	D	4	Total Cd 4 4	0	0
2	E	4	Total Cd 4 4	0	0
2	F	5	Total Cd 5 5	0	0
2	G	4	Total Cd 4 4	0	0
2	H	3	Total Cd 3 3	0	0

3 Residue-property plots

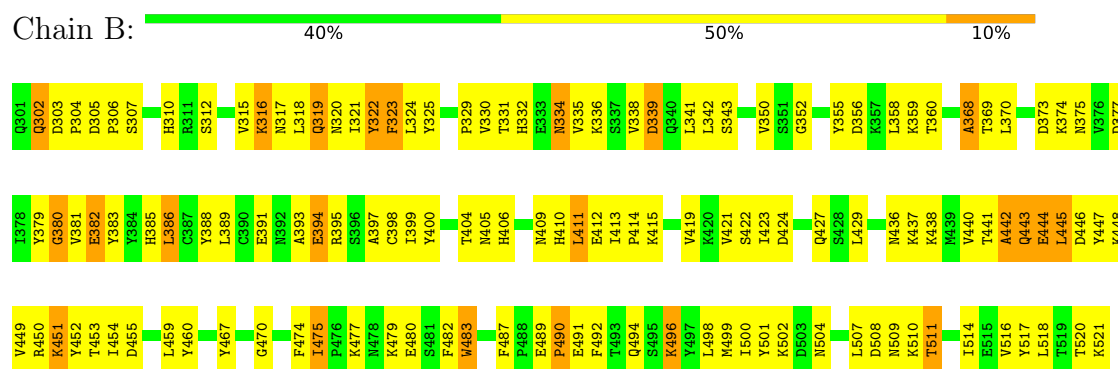
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

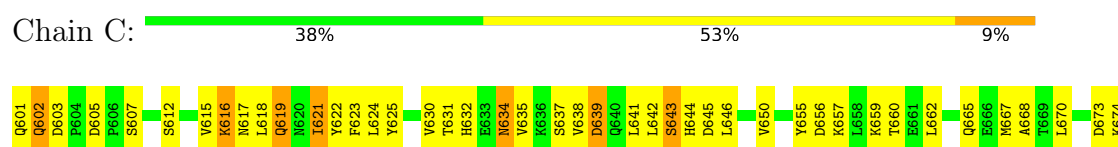
• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)



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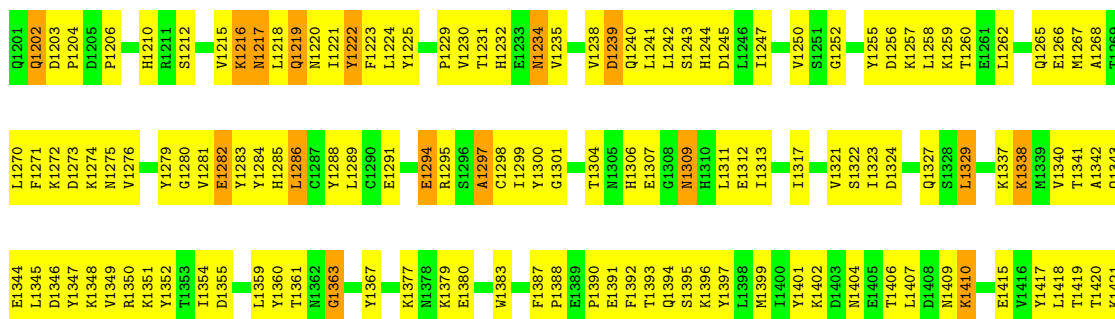
• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain D: 37% 53% 10%



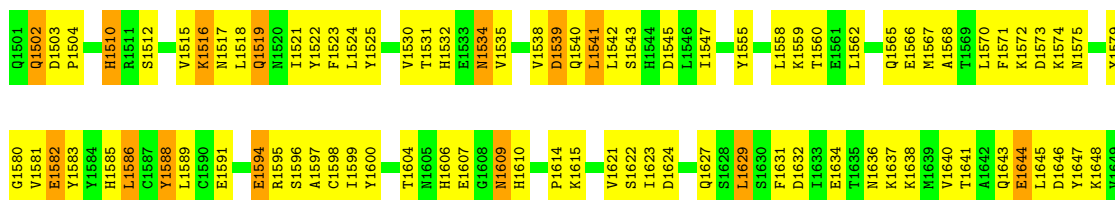
• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

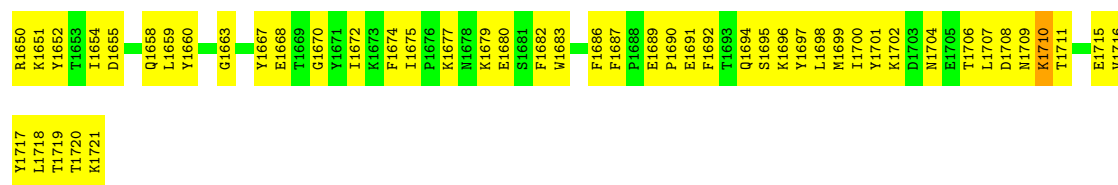
Chain E: 39% 53% 7%



• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

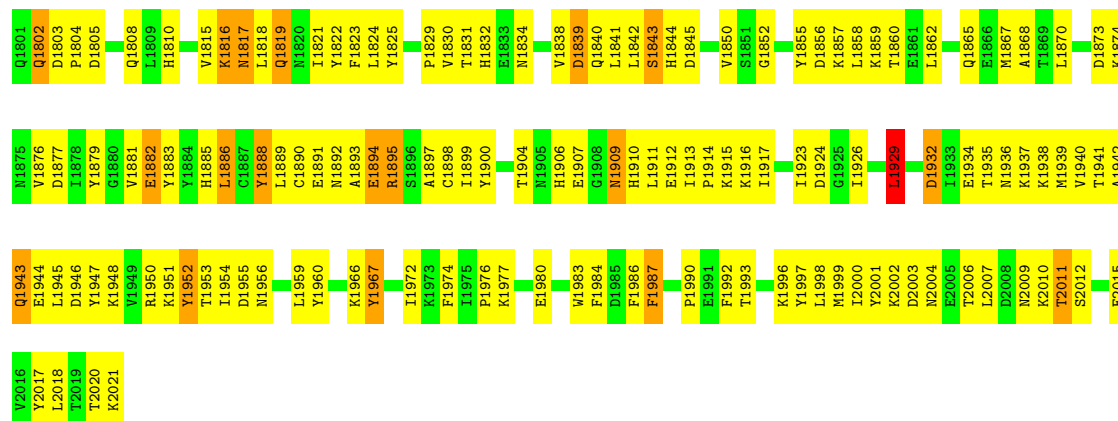
Chain F: 38% 55% 7%





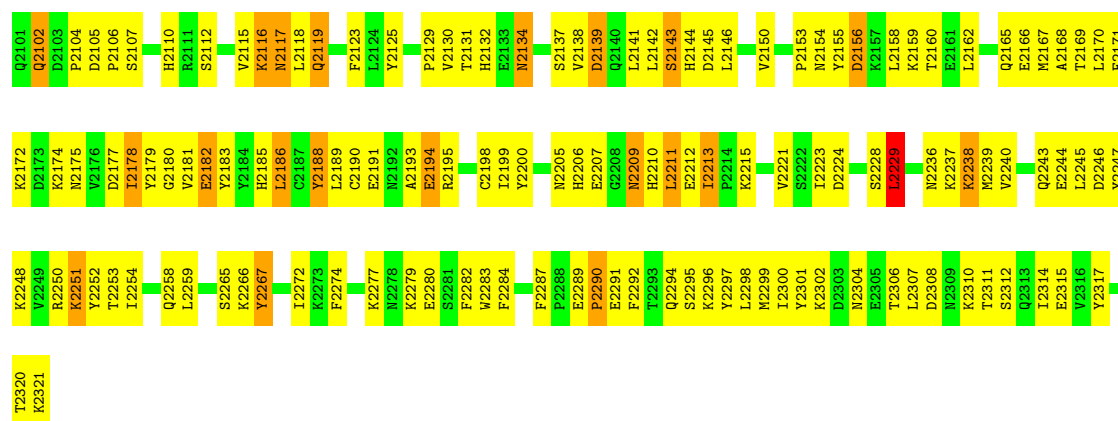
• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain G: 37% 54% 8%



• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain H: 39% 52% 9%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.23Å 226.23Å 81.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.90	Depositor
% Data completeness (in resolution range)	77.0 (20.00-3.90)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14616	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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:
CD

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	0.58	0/1865	1.09	18/2522 (0.7%)
1	B	0.57	0/1865	1.07	16/2522 (0.6%)
1	C	0.52	0/1865	1.03	11/2522 (0.4%)
1	D	0.53	0/1865	1.07	15/2522 (0.6%)
1	E	0.53	0/1865	1.02	10/2522 (0.4%)
1	F	0.56	0/1865	1.05	12/2522 (0.5%)
1	G	0.49	0/1865	1.09	11/2522 (0.4%)
1	H	0.51	0/1865	1.04	12/2522 (0.5%)
All	All	0.54	0/14920	1.06	105/20176 (0.5%)

There are no bond length outliers.

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1280	GLY	N-CA-C	7.98	122.63	110.18
1	F	1521	ILE	N-CA-C	-7.97	104.96	111.81
1	F	1594	GLU	N-CA-C	-7.77	98.38	110.42
1	G	1839	ASP	N-CA-C	-7.66	98.88	110.14
1	D	1011	LEU	N-CA-C	7.59	119.60	110.19
1	G	1911	LEU	N-CA-C	7.44	120.62	110.35
1	H	2238	LYS	N-CA-C	-7.41	103.28	111.36
1	G	1893	ALA	N-CA-C	7.31	120.69	108.20
1	C	639	ASP	N-CA-C	-7.17	98.84	109.81
1	D	1029	LEU	N-CA-C	7.15	117.96	107.88
1	B	438	LYS	N-CA-C	-7.10	103.48	111.07
1	E	1294	GLU	N-CA-C	-7.08	100.32	110.59
1	D	939	ASP	N-CA-C	-7.08	99.12	109.18
1	B	393	ALA	N-CA-C	7.08	120.27	108.73
1	D	921	ILE	N-CA-C	-7.06	105.90	112.96
1	G	1803	ASP	CA-C-N	7.05	127.01	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1803	ASP	C-N-CA	7.05	127.01	120.03
1	B	303	ASP	CA-C-N	7.00	126.93	120.21
1	B	303	ASP	C-N-CA	7.00	126.93	120.21
1	A	94	GLU	N-CA-C	-6.94	100.53	110.59
1	G	1894	GLU	N-CA-C	-6.94	99.00	110.17
1	H	2211	LEU	N-CA-C	6.74	118.55	110.19
1	A	111	LEU	N-CA-C	6.71	120.31	110.59
1	D	994	GLU	N-CA-C	-6.68	99.42	110.17
1	A	129	LEU	N-CA-C	6.66	117.27	107.88
1	F	1663	GLY	CA-C-N	6.66	126.62	119.76
1	F	1663	GLY	C-N-CA	6.66	126.62	119.76
1	E	1239	ASP	N-CA-C	-6.57	99.59	109.96
1	F	1539	ASP	N-CA-C	-6.54	100.53	109.95
1	C	621	ILE	N-CA-C	-6.50	104.69	111.58
1	E	1338	LYS	N-CA-C	-6.29	104.52	111.82
1	A	138	LYS	N-CA-C	-6.27	104.33	112.23
1	B	394	GLU	N-CA-C	-6.25	100.73	110.42
1	B	489	GLU	N-CA-C	-6.24	101.21	110.20
1	D	1038	LYS	N-CA-C	-6.21	104.50	111.28
1	E	1203	ASP	CA-C-N	6.18	126.15	120.03
1	E	1203	ASP	C-N-CA	6.18	126.15	120.03
1	G	1987	PHE	CA-C-N	6.16	126.12	120.21
1	G	1987	PHE	C-N-CA	6.16	126.12	120.21
1	H	2194	GLU	N-CA-C	-6.15	101.42	110.52
1	A	163	GLY	CA-C-N	6.08	126.04	119.78
1	A	163	GLY	C-N-CA	6.08	126.04	119.78
1	H	2312	SER	N-CA-C	6.05	118.51	110.53
1	B	511	THR	N-CA-C	6.03	120.80	113.38
1	B	380	GLY	N-CA-C	6.02	120.56	110.56
1	A	142	ALA	N-CA-C	-5.97	104.77	111.28
1	D	1111	THR	N-CA-C	5.97	120.72	113.38
1	D	993	ALA	N-CA-C	5.96	118.64	108.02
1	F	1675	ILE	CA-C-N	5.96	125.72	119.76
1	F	1675	ILE	C-N-CA	5.96	125.72	119.76
1	F	1503	ASP	CA-C-N	5.85	125.82	120.03
1	F	1503	ASP	C-N-CA	5.85	125.82	120.03
1	A	113	ILE	N-CA-C	5.84	114.25	107.89
1	H	2229	LEU	N-CA-C	5.82	116.09	107.88
1	D	903	ASP	CA-C-N	5.81	126.14	119.92
1	D	903	ASP	C-N-CA	5.81	126.14	119.92
1	G	1938	LYS	N-CA-C	-5.79	105.05	111.36
1	C	711	LEU	N-CA-C	5.78	118.44	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1929	LEU	N-CA-C	5.74	115.97	107.88
1	B	442	ALA	N-CA-C	-5.70	104.44	111.33
1	A	141	THR	N-CA-C	-5.68	101.88	110.28
1	B	496	LYS	N-CA-C	5.67	118.22	111.71
1	C	693	ALA	N-CA-C	5.65	117.90	108.02
1	D	1089	GLU	N-CA-C	-5.59	102.15	110.20
1	H	2178	ILE	N-CA-C	5.59	116.00	108.17
1	B	411	LEU	N-CA-C	5.58	118.70	109.94
1	F	1629	LEU	N-CA-C	5.58	116.44	108.74
1	F	1638	LYS	N-CA-C	-5.57	105.31	111.71
1	B	339	ASP	N-CA-C	-5.55	101.18	109.96
1	H	2193	ALA	N-CA-C	5.54	118.05	107.75
1	D	1120	THR	N-CA-C	-5.53	105.79	112.54
1	A	175	ILE	CA-C-N	5.52	125.99	120.14
1	A	175	ILE	C-N-CA	5.52	125.99	120.14
1	A	187	PHE	CA-C-N	5.52	125.72	120.31
1	A	187	PHE	C-N-CA	5.52	125.72	120.31
1	A	80	GLY	N-CA-C	5.50	118.76	110.18
1	C	740	VAL	N-CA-C	5.44	117.40	108.97
1	H	2156	ASP	N-CA-C	-5.43	106.03	113.30
1	C	775	ILE	CA-C-N	5.42	125.18	119.76
1	C	775	ILE	C-N-CA	5.42	125.18	119.76
1	E	1363	GLY	CA-C-N	5.42	125.42	119.89
1	E	1363	GLY	C-N-CA	5.42	125.42	119.89
1	C	603	ASP	CA-C-N	5.40	126.59	119.84
1	C	603	ASP	C-N-CA	5.40	126.59	119.84
1	E	1329	LEU	N-CA-C	5.40	115.67	108.38
1	G	2011	THR	N-CA-C	5.38	120.00	113.38
1	E	1276	VAL	N-CA-C	5.28	115.26	108.82
1	A	3	ASP	CA-C-N	5.28	126.02	120.11
1	A	3	ASP	C-N-CA	5.28	126.02	120.11
1	A	183	TRP	N-CA-C	5.24	116.25	108.60
1	D	955	TYR	N-CA-C	5.20	116.43	108.52
1	H	2158	LEU	N-CA-C	5.20	116.51	107.93
1	C	741	THR	N-CA-C	-5.20	101.95	109.59
1	H	2139	ASP	N-CA-C	-5.14	102.58	110.14
1	B	475	ILE	CA-C-N	5.09	125.25	119.90
1	B	475	ILE	C-N-CA	5.09	125.25	119.90
1	B	352	GLY	N-CA-C	-5.09	101.95	112.34
1	C	694	GLU	N-CA-C	-5.08	101.87	109.95
1	F	1510	HIS	N-CA-C	-5.06	103.37	110.50
1	B	483	TRP	N-CA-C	5.06	116.49	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ILE	N-CA-C	5.05	115.39	108.12
1	H	2190	CYS	N-CA-C	-5.04	102.05	110.17
1	D	1075	ILE	CA-C-N	5.03	125.19	119.90
1	D	1075	ILE	C-N-CA	5.03	125.19	119.90
1	H	2213	ILE	N-CA-C	5.02	113.36	107.89

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	1823	0	1778	171	0
1	B	1823	0	1775	158	0
1	C	1823	0	1775	160	0
1	D	1823	0	1775	167	0
1	E	1823	0	1775	159	0
1	F	1823	0	1775	161	0
1	G	1823	0	1775	167	0
1	H	1823	0	1775	174	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	5	0	0	0	0
2	G	4	0	0	0	0
2	H	3	0	0	0	0
All	All	14616	0	14203	1270	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 44.

All (1270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:GLU:HB3	1:D:991:GLU:HB3	1.36	1.03
1:C:619:GLN:H	1:C:619:GLN:NE2	1.55	1.03
1:H:2119:GLN:H	1:H:2119:GLN:NE2	1.54	1.03
1:E:1219:GLN:H	1:E:1219:GLN:NE2	1.57	1.02
1:E:1291:GLU:HB3	1:G:1891:GLU:HB3	1.38	1.02
1:A:19:GLN:H	1:A:19:GLN:NE2	1.58	1.01
1:H:2102:GLN:H	1:H:2102:GLN:NE2	1.59	0.99
1:B:479:LYS:HG3	1:B:480:GLU:H	1.27	0.98
1:F:1591:GLU:HB3	1:H:2191:GLU:HB3	1.41	0.98
1:C:754:ILE:HG12	1:C:759:LEU:HB3	1.42	0.98
1:A:19:GLN:H	1:A:19:GLN:HE21	1.05	0.98
1:G:1819:GLN:H	1:G:1819:GLN:NE2	1.60	0.98
1:C:619:GLN:H	1:C:619:GLN:HE21	1.04	0.97
1:H:2119:GLN:H	1:H:2119:GLN:HE21	1.09	0.96
1:D:959:LYS:HB2	1:D:989:LEU:HD21	1.45	0.95
1:A:91:GLU:HB3	1:C:691:GLU:HB3	1.46	0.95
1:B:359:LYS:HB2	1:B:389:LEU:HD21	1.46	0.94
1:H:2254:ILE:HG12	1:H:2259:LEU:HB3	1.48	0.94
1:B:338:VAL:HG23	1:B:339:ASP:H	1.33	0.93
1:G:1838:VAL:HG23	1:G:1839:ASP:H	1.31	0.93
1:D:919:GLN:NE2	1:D:919:GLN:H	1.66	0.93
1:F:1581:VAL:H	1:F:1643:GLN:HE21	1.16	0.92
1:G:1819:GLN:H	1:G:1819:GLN:HE21	0.99	0.92
1:E:1354:ILE:HG12	1:E:1359:LEU:HB3	1.51	0.92
1:B:319:GLN:H	1:B:319:GLN:HE21	0.97	0.92
1:F:1519:GLN:H	1:F:1519:GLN:HE21	1.19	0.91
1:E:1219:GLN:H	1:E:1219:GLN:HE21	1.03	0.90
1:F:1519:GLN:H	1:F:1519:GLN:NE2	1.68	0.90
1:B:319:GLN:H	1:B:319:GLN:NE2	1.69	0.90
1:F:1654:ILE:HG12	1:F:1659:LEU:HB3	1.56	0.88
1:A:59:LYS:HB2	1:A:89:LEU:HD21	1.54	0.88
1:H:2102:GLN:H	1:H:2102:GLN:HE21	1.20	0.88
1:B:319:GLN:HE21	1:B:319:GLN:N	1.74	0.86
1:F:1581:VAL:H	1:F:1643:GLN:NE2	1.73	0.86
1:B:454:ILE:HG12	1:B:459:LEU:HB3	1.57	0.85
1:G:1996:LYS:HD3	1:G:1997:TYR:N	1.92	0.84
1:H:2131:THR:HG22	1:H:2179:TYR:CD1	2.12	0.84
1:H:2102:GLN:HE21	1:H:2102:GLN:N	1.75	0.84
1:H:2296:LYS:HD3	1:H:2297:TYR:N	1.93	0.83
1:G:1859:LYS:HB2	1:G:1889:LEU:HD21	1.59	0.83
1:F:1559:LYS:HB2	1:F:1589:LEU:HD21	1.59	0.82
1:B:338:VAL:HG23	1:B:339:ASP:N	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG23	1:A:39:ASP:H	1.44	0.82
1:C:625:TYR:CE2	1:C:750:ARG:HD2	2.15	0.82
1:D:925:TYR:CE2	1:D:1050:ARG:HD2	2.15	0.82
1:G:1858:LEU:HD12	1:G:1897:ALA:O	1.78	0.81
1:A:38:VAL:HG23	1:A:39:ASP:N	1.94	0.81
1:B:325:TYR:CE2	1:B:450:ARG:HD2	2.16	0.81
1:A:179:LYS:HG3	1:A:180:GLU:H	1.45	0.81
1:B:379:TYR:CE2	1:B:444:GLU:HG3	2.15	0.81
1:B:383:TYR:CE1	1:B:398:CYS:HB2	2.15	0.81
1:D:981:VAL:H	1:D:1043:GLN:NE2	1.79	0.81
1:H:2130:VAL:HG21	1:H:2182:GLU:HB3	1.62	0.80
1:H:2159:LYS:HB2	1:H:2189:LEU:HD21	1.63	0.80
1:A:196:LYS:HD3	1:A:196:LYS:C	2.07	0.79
1:F:1562:LEU:HD12	1:F:1568:ALA:HA	1.65	0.79
1:H:2237:LYS:HB2	1:H:2240:VAL:HG12	1.63	0.79
1:B:373:ASP:C	1:B:374:LYS:HD2	2.08	0.78
1:E:1351:LYS:HE2	1:E:1355:ASP:OD2	1.83	0.78
1:G:1838:VAL:HG23	1:G:1839:ASP:N	1.98	0.78
1:D:1037:LYS:HB2	1:D:1040:VAL:HG12	1.65	0.78
1:B:400:TYR:CE2	1:B:499:MET:HG2	2.17	0.78
1:D:962:LEU:HD12	1:D:968:ALA:HA	1.64	0.78
1:H:2195:ARG:NH1	1:H:2195:ARG:HB3	1.99	0.78
1:D:973:ASP:C	1:D:974:LYS:HD2	2.08	0.78
1:E:1291:GLU:HB3	1:G:1891:GLU:CB	2.14	0.78
1:A:154:ILE:HG12	1:A:159:LEU:HB3	1.65	0.77
1:C:616:LYS:HD3	1:C:791:GLU:HG2	1.65	0.77
1:E:1295:ARG:HB3	1:E:1295:ARG:NH1	2.00	0.77
1:F:1709:ASN:CG	1:F:1710:LYS:H	1.92	0.77
1:B:391:GLU:HB3	1:D:991:GLU:CB	2.15	0.77
1:F:1538:VAL:HG23	1:F:1539:ASP:H	1.48	0.77
1:E:1273:ASP:C	1:E:1274:LYS:HD2	2.10	0.76
1:G:1819:GLN:HE21	1:G:1819:GLN:N	1.79	0.76
1:H:2254:ILE:HA	1:H:2259:LEU:H	1.50	0.76
1:A:15:VAL:HG11	1:A:18:LEU:HD13	1.68	0.76
1:F:1560:THR:HA	1:F:1599:ILE:O	1.86	0.76
1:E:1396:LYS:HD3	1:E:1397:TYR:N	2.01	0.76
1:H:2116:LYS:HE2	1:H:2292:PHE:H	1.49	0.76
1:F:1516:LYS:HG3	1:F:1517:ASN:H	1.50	0.76
1:D:919:GLN:H	1:D:919:GLN:HE21	1.29	0.76
1:F:1679:LYS:HG3	1:F:1680:GLU:H	1.49	0.76
1:E:1225:TYR:CE2	1:E:1350:ARG:HD2	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1516:LYS:HE2	1:F:1691:GLU:HA	1.66	0.76
1:A:196:LYS:HD3	1:A:197:TYR:N	2.00	0.75
1:E:1238:VAL:HG23	1:E:1239:ASP:N	2.01	0.75
1:F:1541:LEU:HG	1:F:1542:LEU:HG	1.69	0.75
1:H:2125:TYR:CE2	1:H:2250:ARG:HD2	2.21	0.75
1:C:659:LYS:HB2	1:C:689:LEU:HD21	1.69	0.75
1:G:1825:TYR:CE2	1:G:1950:ARG:HD2	2.22	0.75
1:G:1882:GLU:HA	1:G:1899:ILE:HG22	1.69	0.75
1:B:391:GLU:CB	1:D:991:GLU:HB3	2.13	0.75
1:C:751:LYS:HE2	1:C:755:ASP:OD2	1.87	0.75
1:H:2138:VAL:HG23	1:H:2139:ASP:H	1.51	0.75
1:A:19:GLN:NE2	1:A:19:GLN:N	2.35	0.74
1:A:30:VAL:HG21	1:A:82:GLU:HB3	1.68	0.74
1:G:1802:GLN:H	1:G:1802:GLN:NE2	1.85	0.74
1:G:1916:LYS:HG2	1:G:1934:GLU:HG2	1.69	0.74
1:H:2115:VAL:HG13	1:H:2292:PHE:HE2	1.52	0.74
1:B:496:LYS:C	1:B:496:LYS:HD3	2.12	0.74
1:E:1291:GLU:CB	1:G:1891:GLU:HB3	2.17	0.74
1:A:73:ASP:C	1:A:74:LYS:HD2	2.13	0.74
1:F:1538:VAL:HG23	1:F:1539:ASP:N	2.02	0.74
1:H:2296:LYS:HD3	1:H:2296:LYS:C	2.12	0.74
1:A:91:GLU:HB3	1:C:691:GLU:CB	2.18	0.73
1:E:1285:HIS:CD2	1:F:1594:GLU:HG2	2.23	0.73
1:E:1219:GLN:HE21	1:E:1219:GLN:N	1.84	0.73
1:B:454:ILE:HA	1:B:459:LEU:H	1.53	0.73
1:E:1219:GLN:NE2	1:E:1219:GLN:N	2.34	0.73
1:E:1282:GLU:HA	1:E:1299:ILE:HG22	1.71	0.73
1:F:1579:TYR:CE2	1:F:1644:GLU:HG3	2.23	0.73
1:H:2131:THR:HG22	1:H:2179:TYR:HD1	1.54	0.73
1:G:1819:GLN:NE2	1:G:1819:GLN:N	2.34	0.72
1:H:2277:LYS:O	1:H:2277:LYS:HD3	1.88	0.72
1:B:334:ASN:HB2	1:B:406:HIS:CD2	2.24	0.72
1:F:1516:LYS:HG3	1:F:1517:ASN:N	2.02	0.72
1:B:335:VAL:O	1:B:375:ASN:HA	1.89	0.72
1:E:1281:VAL:H	1:E:1343:GLN:NE2	1.88	0.72
1:E:1291:GLU:HG2	1:G:1891:GLU:OE1	1.90	0.72
1:E:1217:ASN:HB3	1:E:1219:GLN:OE1	1.88	0.72
1:H:2138:VAL:HG23	1:H:2139:ASP:N	2.03	0.72
1:C:619:GLN:HE21	1:C:619:GLN:N	1.84	0.71
1:A:19:GLN:HE21	1:A:19:GLN:N	1.83	0.71
1:D:916:LYS:HG3	1:D:917:ASN:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1862:LEU:HD12	1:G:1868:ALA:HA	1.72	0.71
1:E:1258:LEU:HD12	1:E:1297:ALA:O	1.90	0.71
1:F:1525:TYR:CE2	1:F:1650:ARG:HD2	2.25	0.71
1:E:1291:GLU:OE1	1:G:1891:GLU:HG2	1.90	0.71
1:A:91:GLU:H	1:C:691:GLU:CD	1.98	0.71
1:C:616:LYS:HE2	1:C:791:GLU:HA	1.72	0.71
1:H:2130:VAL:CG2	1:H:2182:GLU:HB3	2.19	0.71
1:A:24:LEU:HD13	1:A:198:LEU:HD21	1.73	0.70
1:C:619:GLN:NE2	1:C:619:GLN:N	2.36	0.70
1:D:956:ASP:O	1:D:957:LYS:HD3	1.89	0.70
1:A:16:LYS:HE2	1:A:192:PHE:H	1.55	0.70
1:D:916:LYS:HG3	1:D:917:ASN:H	1.56	0.70
1:E:1281:VAL:H	1:E:1343:GLN:HE21	1.38	0.70
1:F:1696:LYS:HD3	1:F:1696:LYS:C	2.15	0.70
1:D:1054:ILE:HG12	1:D:1059:LEU:HB3	1.74	0.70
1:C:673:ASP:C	1:C:674:LYS:HD2	2.16	0.70
1:D:979:TYR:CE2	1:D:1044:GLU:HG3	2.26	0.70
1:D:1079:LYS:HG3	1:D:1080:GLU:H	1.56	0.70
1:H:2134:ASN:HB2	1:H:2206:HIS:CD2	2.26	0.70
1:B:338:VAL:CG2	1:B:339:ASP:H	2.05	0.70
1:H:2221:VAL:HB	1:H:2229:LEU:HD12	1.73	0.69
1:A:2:GLN:H	1:A:2:GLN:NE2	1.90	0.69
1:H:2119:GLN:HE21	1:H:2119:GLN:N	1.87	0.69
1:E:1230:VAL:HG13	1:E:1255:TYR:OH	1.93	0.69
1:E:1234:ASN:HB2	1:E:1306:HIS:CD2	2.27	0.69
1:A:91:GLU:HG2	1:C:691:GLU:OE1	1.92	0.69
1:B:312:SER:HB3	1:B:487:PHE:CE2	2.28	0.69
1:E:1259:LYS:HB2	1:E:1289:LEU:HD21	1.75	0.69
1:G:1877:ASP:OD2	1:G:1906:HIS:HA	1.93	0.69
1:G:1816:LYS:HE2	1:G:1992:PHE:H	1.58	0.69
1:C:681:VAL:H	1:C:743:GLN:HE21	1.39	0.69
1:F:1519:GLN:NE2	1:F:1519:GLN:N	2.40	0.69
1:A:150:ARG:O	1:A:151:LYS:C	2.36	0.69
1:F:1558:LEU:HD12	1:F:1597:ALA:O	1.92	0.69
1:G:1977:LYS:HB2	1:G:2011:THR:HB	1.75	0.69
1:B:451:LYS:HE2	1:B:455:ASP:OD2	1.93	0.69
1:H:2112:SER:HB3	1:H:2287:PHE:CE2	2.27	0.69
1:C:631:THR:HG22	1:C:679:TYR:CD1	2.29	0.68
1:G:2007:LEU:HD12	1:G:2007:LEU:O	1.93	0.68
1:E:1283:TYR:CE1	1:E:1298:CYS:HB2	2.29	0.68
1:E:1379:LYS:HG3	1:E:1380:GLU:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2181:VAL:H	1:H:2243:GLN:HE21	1.39	0.68
1:G:1817:ASN:HB3	1:G:1819:GLN:OE1	1.94	0.67
1:A:38:VAL:CG2	1:A:39:ASP:H	2.07	0.67
1:D:1051:LYS:HE2	1:D:1055:ASP:OD2	1.93	0.67
1:H:2179:TYR:CD2	1:H:2244:GLU:HG3	2.29	0.67
1:B:370:LEU:HD23	1:B:370:LEU:O	1.95	0.67
1:D:916:LYS:HE2	1:D:1092:PHE:H	1.59	0.67
1:C:634:ASN:HB2	1:C:706:HIS:CD2	2.30	0.67
1:E:1300:TYR:CE2	1:E:1399:MET:HG2	2.28	0.67
1:G:1805:ASP:H	1:G:1808:GLN:NE2	1.92	0.67
1:H:2243:GLN:HG3	1:H:2301:TYR:CD1	2.30	0.67
1:A:25:TYR:CE2	1:A:150:ARG:HD2	2.29	0.67
1:A:100:TYR:CE2	1:A:199:MET:HG2	2.31	0.66
1:C:698:CYS:O	1:C:699:ILE:HG23	1.95	0.66
1:F:1610:HIS:CD2	1:F:1636:ASN:HB3	2.30	0.66
1:H:2267:TYR:CD1	1:H:2267:TYR:N	2.63	0.66
1:B:450:ARG:O	1:B:451:LYS:C	2.38	0.66
1:A:83:TYR:HB2	1:A:194:GLN:HE21	1.60	0.66
1:D:985:HIS:CD2	1:D:986:LEU:HG	2.31	0.66
1:E:1291:GLU:CD	1:G:1891:GLU:H	2.03	0.66
1:H:2307:LEU:HD12	1:H:2307:LEU:O	1.95	0.66
1:B:437:LYS:HB2	1:B:440:VAL:HG12	1.78	0.66
1:F:1709:ASN:CG	1:F:1710:LYS:N	2.50	0.66
1:B:325:TYR:CD2	1:B:450:ARG:HD2	2.30	0.66
1:D:931:THR:HG22	1:D:979:TYR:CD1	2.31	0.66
1:E:1238:VAL:HG23	1:E:1239:ASP:H	1.59	0.66
1:B:316:LYS:HD3	1:B:491:GLU:HG2	1.78	0.66
1:A:143:GLN:O	1:A:144:GLU:C	2.39	0.66
1:B:507:LEU:O	1:B:507:LEU:HD12	1.96	0.65
1:F:1707:LEU:HD12	1:F:1707:LEU:O	1.96	0.65
1:A:2:GLN:H	1:A:2:GLN:HE21	1.42	0.65
1:B:316:LYS:HG3	1:B:317:ASN:H	1.60	0.65
1:D:904:PRO:HB3	1:D:1083:TRP:CZ2	2.31	0.65
1:B:316:LYS:HG3	1:B:317:ASN:N	2.11	0.65
1:D:1045:LEU:O	1:D:1049:VAL:HG23	1.96	0.65
1:A:179:LYS:HG3	1:A:180:GLU:N	2.12	0.65
1:D:1043:GLN:HG3	1:D:1101:TYR:CD1	2.31	0.65
1:G:1996:LYS:HD3	1:G:1996:LYS:C	2.21	0.65
1:E:1396:LYS:HD3	1:E:1396:LYS:C	2.21	0.65
1:C:674:LYS:HD2	1:C:674:LYS:N	2.11	0.65
1:D:915:VAL:HA	1:D:1090:PRO:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:VAL:HG13	1:A:214:ILE:HG22	1.78	0.65
1:C:700:TYR:CE2	1:C:799:MET:HG2	2.31	0.65
1:A:137:LYS:HB2	1:A:140:VAL:HG12	1.79	0.65
1:C:602:GLN:H	1:C:602:GLN:NE2	1.94	0.65
1:F:1519:GLN:O	1:F:1522:TYR:HB3	1.97	0.65
1:C:739:MET:HE3	1:C:806:THR:HG22	1.78	0.64
1:B:360:THR:HA	1:B:399:ILE:O	1.98	0.64
1:B:391:GLU:HG2	1:D:991:GLU:OE1	1.97	0.64
1:B:479:LYS:HG3	1:B:480:GLU:N	2.06	0.64
1:H:2119:GLN:NE2	1:H:2119:GLN:N	2.37	0.64
1:A:81:VAL:H	1:A:143:GLN:NE2	1.95	0.64
1:A:83:TYR:CE1	1:A:98:CYS:HB2	2.32	0.64
1:C:681:VAL:H	1:C:743:GLN:NE2	1.96	0.64
1:D:1043:GLN:HG3	1:D:1101:TYR:CE1	2.32	0.64
1:G:1860:THR:HA	1:G:1899:ILE:O	1.96	0.64
1:B:500:ILE:HG13	1:B:501:TYR:CD2	2.31	0.64
1:C:820:THR:O	1:C:821:LYS:C	2.40	0.64
1:F:1573:ASP:C	1:F:1574:LYS:HD2	2.23	0.64
1:A:16:LYS:O	1:A:18:LEU:N	2.31	0.64
1:B:316:LYS:HE2	1:B:491:GLU:HA	1.80	0.64
1:C:779:LYS:HG3	1:C:780:GLU:H	1.63	0.64
1:E:1294:GLU:HG2	1:F:1585:HIS:CD2	2.32	0.64
1:F:1535:VAL:O	1:F:1575:ASN:HA	1.98	0.64
1:H:2112:SER:HB3	1:H:2287:PHE:CD2	2.32	0.64
1:D:1029:LEU:C	1:D:1029:LEU:HD12	2.23	0.64
1:E:1359:LEU:HG	1:E:1360:TYR:CD2	2.33	0.64
1:E:1291:GLU:H	1:G:1891:GLU:CD	2.06	0.64
1:F:1670:GLY:HA3	1:F:1718:LEU:HD23	1.80	0.63
1:H:2116:LYS:HG3	1:H:2117:ASN:N	2.12	0.63
1:E:1420:THR:O	1:E:1421:LYS:C	2.41	0.63
1:F:1547:ILE:HD13	1:F:1589:LEU:HD22	1.80	0.63
1:G:1829:PRO:HD3	1:G:1947:TYR:CZ	2.32	0.63
1:H:2142:LEU:C	1:H:2144:HIS:H	2.06	0.63
1:A:79:TYR:CE2	1:A:144:GLU:HG3	2.33	0.63
1:D:931:THR:HG22	1:D:979:TYR:HD1	1.63	0.63
1:G:1910:HIS:CD2	1:G:1936:ASN:HB3	2.34	0.63
1:H:2300:ILE:HG13	1:H:2301:TYR:CD2	2.33	0.63
1:C:638:VAL:HG23	1:C:639:ASP:H	1.63	0.63
1:D:1072:ILE:HB	1:D:1086:PHE:CE2	2.34	0.63
1:A:177:LYS:HD3	1:A:177:LYS:O	1.99	0.63
1:B:391:GLU:OE1	1:D:991:GLU:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:935:VAL:O	1:D:975:ASN:HA	1.99	0.63
1:F:1570:LEU:O	1:F:1570:LEU:HD23	1.98	0.63
1:G:1881:VAL:H	1:G:1943:GLN:HE21	1.46	0.63
1:A:95:ARG:HB3	1:A:95:ARG:NH1	2.14	0.62
1:F:1583:TYR:CE1	1:F:1598:CYS:HB2	2.34	0.62
1:A:45:ASP:O	1:A:46:LEU:HD23	1.98	0.62
1:B:383:TYR:CE1	1:B:398:CYS:CB	2.82	0.62
1:E:1225:TYR:CD2	1:E:1350:ARG:HD2	2.35	0.62
1:G:1804:PRO:HD3	1:G:1983:TRP:CD1	2.34	0.62
1:B:470:GLY:HA2	1:B:517:TYR:O	2.00	0.62
1:G:1855:TYR:C	1:G:1895:ARG:HH12	2.08	0.62
1:A:38:VAL:CG2	1:A:39:ASP:N	2.62	0.62
1:C:612:SER:HB3	1:C:787:PHE:CE2	2.34	0.62
1:D:925:TYR:CD2	1:D:1050:ARG:HD2	2.34	0.62
1:F:1650:ARG:O	1:F:1651:LYS:C	2.41	0.62
1:C:777:LYS:O	1:C:777:LYS:HD3	1.98	0.62
1:F:1525:TYR:CD2	1:F:1650:ARG:HD2	2.35	0.62
1:B:319:GLN:NE2	1:B:319:GLN:N	2.38	0.62
1:D:959:LYS:HB2	1:D:989:LEU:CD2	2.27	0.62
1:D:974:LYS:HD2	1:D:974:LYS:N	2.14	0.62
1:E:1229:PRO:HD3	1:E:1347:TYR:CE2	2.34	0.62
1:G:1977:LYS:CB	1:G:2011:THR:HB	2.30	0.62
1:D:981:VAL:H	1:D:1043:GLN:HE21	1.45	0.61
1:E:1223:PHE:CE2	1:F:1595:ARG:NH2	2.67	0.61
1:E:1252:GLY:HA3	1:E:1255:TYR:CZ	2.35	0.61
1:F:1583:TYR:HB2	1:F:1694:GLN:HE21	1.65	0.61
1:C:800:ILE:HG13	1:C:801:TYR:CD2	2.34	0.61
1:F:1696:LYS:HD3	1:F:1697:TYR:N	2.16	0.61
1:C:743:GLN:O	1:C:744:GLU:C	2.41	0.61
1:F:1538:VAL:CG2	1:F:1539:ASP:H	2.13	0.61
1:F:1609:ASN:O	1:F:1637:LYS:HA	2.00	0.61
1:C:630:VAL:HG21	1:C:682:GLU:HB3	1.83	0.61
1:E:1279:TYR:CE2	1:E:1344:GLU:HG3	2.36	0.61
1:A:115:LYS:HD3	1:A:210:LYS:NZ	2.15	0.61
1:G:1943:GLN:OE1	1:G:2001:TYR:HB3	2.01	0.61
1:G:1838:VAL:CG2	1:G:1839:ASP:H	2.08	0.61
1:C:638:VAL:HG23	1:C:639:ASP:N	2.16	0.61
1:D:970:LEU:O	1:D:970:LEU:HD23	2.00	0.61
1:G:1879:TYR:CE2	1:G:1944:GLU:HG3	2.35	0.61
1:C:796:LYS:HD3	1:C:796:LYS:C	2.26	0.61
1:E:1216:LYS:HG3	1:E:1217:ASN:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1650:ARG:O	1:F:1654:ILE:HG13	1.99	0.61
1:E:1279:TYR:CD2	1:E:1344:GLU:HG3	2.35	0.61
1:B:492:PHE:CD1	1:B:492:PHE:C	2.79	0.61
1:C:743:GLN:HG3	1:C:801:TYR:CD1	2.36	0.61
1:B:359:LYS:HB2	1:B:389:LEU:CD2	2.26	0.60
1:G:1829:PRO:HD3	1:G:1947:TYR:CE2	2.36	0.60
1:H:2160:THR:HG23	1:H:2160:THR:O	2.01	0.60
1:B:395:ARG:NH1	1:B:395:ARG:HB3	2.16	0.60
1:C:745:LEU:O	1:C:746:ASP:C	2.43	0.60
1:F:1679:LYS:HG3	1:F:1680:GLU:N	2.16	0.60
1:A:60:THR:HA	1:A:99:ILE:O	2.01	0.60
1:E:1229:PRO:HD3	1:E:1347:TYR:CZ	2.37	0.60
1:G:1860:THR:HG23	1:G:1860:THR:O	2.01	0.60
1:H:2179:TYR:CE2	1:H:2244:GLU:HG3	2.37	0.60
1:H:2102:GLN:NE2	1:H:2102:GLN:N	2.35	0.60
1:D:1000:TYR:CE2	1:D:1099:MET:HG2	2.36	0.60
1:D:1061:THR:O	1:D:1063:GLY:N	2.34	0.60
1:G:1915:LYS:HE3	1:G:2010:LYS:HD3	1.82	0.60
1:A:34:ASN:HB2	1:A:106:HIS:CD2	2.37	0.60
1:B:520:THR:O	1:B:521:LYS:C	2.43	0.60
1:G:1929:LEU:C	1:G:1929:LEU:HD12	2.27	0.60
1:A:91:GLU:OE1	1:C:691:GLU:HG2	2.01	0.60
1:B:509:ASN:CG	1:B:510:LYS:N	2.60	0.60
1:B:429:LEU:C	1:B:429:LEU:HD12	2.26	0.59
1:E:1409:ASN:CG	1:E:1410:LYS:H	2.08	0.59
1:F:1677:LYS:HB2	1:F:1711:THR:HB	1.84	0.59
1:B:323:PHE:O	1:B:324:LEU:C	2.45	0.59
1:C:616:LYS:HG3	1:C:617:ASN:N	2.17	0.59
1:C:685:HIS:CD2	1:D:994:GLU:HG2	2.37	0.59
1:G:1804:PRO:HD3	1:G:1983:TRP:NE1	2.18	0.59
1:B:322:TYR:O	1:B:323:PHE:C	2.45	0.59
1:D:1096:LYS:HD3	1:D:1096:LYS:C	2.26	0.59
1:A:62:LEU:HD12	1:A:68:ALA:HA	1.83	0.59
1:B:316:LYS:HE2	1:B:492:PHE:H	1.66	0.59
1:D:916:LYS:HD3	1:D:1091:GLU:HG2	1.83	0.59
1:F:1591:GLU:HB3	1:H:2191:GLU:CB	2.26	0.59
1:G:1841:LEU:HG	1:G:1842:LEU:HG	1.84	0.59
1:G:1951:LYS:HE2	1:G:1955:ASP:OD2	2.03	0.59
1:E:1409:ASN:CG	1:E:1410:LYS:N	2.60	0.59
1:A:12:SER:HB3	1:A:187:PHE:CE2	2.38	0.59
1:A:60:THR:HG23	1:A:60:THR:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1885:HIS:CD2	1:H:2194:GLU:HG2	2.38	0.59
1:C:754:ILE:CG1	1:C:759:LEU:HB3	2.25	0.59
1:C:677:ASP:OD1	1:C:706:HIS:HD2	1.84	0.59
1:C:602:GLN:N	1:C:602:GLN:HE21	2.00	0.59
1:B:330:VAL:HG21	1:B:382:GLU:HB3	1.85	0.59
1:D:934:ASN:OD1	1:D:975:ASN:HB3	2.02	0.59
1:E:1350:ARG:O	1:E:1351:LYS:C	2.45	0.59
1:F:1581:VAL:N	1:F:1643:GLN:NE2	2.48	0.59
1:G:1873:ASP:C	1:G:1874:LYS:HD2	2.28	0.59
1:D:904:PRO:HD3	1:D:1083:TRP:CE2	2.38	0.58
1:G:1945:LEU:HD12	1:G:1974:PHE:HE2	1.68	0.58
1:A:94:GLU:HG2	1:B:385:HIS:CD2	2.38	0.58
1:D:929:PRO:HD3	1:D:1047:TYR:CZ	2.38	0.58
1:D:932:HIS:CE1	1:D:950:VAL:HB	2.38	0.58
1:D:942:LEU:O	1:D:944:HIS:N	2.35	0.58
1:D:983:TYR:CE1	1:D:998:CYS:CB	2.87	0.58
1:F:1534:ASN:HB2	1:F:1606:HIS:CD2	2.38	0.58
1:D:1117:TYR:O	1:D:1118:LEU:HD23	2.04	0.58
1:G:1870:LEU:O	1:G:1874:LYS:HD3	2.04	0.58
1:G:1937:LYS:HB2	1:G:1940:VAL:HG12	1.84	0.58
1:D:960:THR:HG23	1:D:960:THR:O	2.03	0.58
1:C:721:VAL:HB	1:C:729:LEU:HD12	1.85	0.58
1:D:977:ASP:OD2	1:D:1006:HIS:HA	2.04	0.58
1:E:1235:VAL:O	1:E:1275:ASN:HA	2.02	0.58
1:F:1594:GLU:O	1:F:1595:ARG:HB2	2.03	0.58
1:E:1304:THR:HG23	1:E:1341:THR:HG22	1.86	0.58
1:G:1862:LEU:HB3	1:G:1867:MET:SD	2.44	0.58
1:G:1967:TYR:CD1	1:G:1967:TYR:N	2.72	0.58
1:H:2141:LEU:HG	1:H:2142:LEU:HG	1.84	0.58
1:A:77:ASP:OD1	1:A:106:HIS:HD2	1.87	0.58
1:D:983:TYR:HB2	1:D:1094:GLN:HE21	1.69	0.57
1:G:1825:TYR:CD2	1:G:1950:ARG:HD2	2.39	0.57
1:A:83:TYR:HB2	1:A:194:GLN:NE2	2.18	0.57
1:C:625:TYR:CD2	1:C:750:ARG:HD2	2.39	0.57
1:C:750:ARG:O	1:C:754:ILE:HG13	2.04	0.57
1:D:1109:ASN:CG	1:D:1110:LYS:N	2.62	0.57
1:E:1217:ASN:HA	1:E:1219:GLN:HE22	1.69	0.57
1:F:1516:LYS:HD3	1:F:1691:GLU:HG2	1.86	0.57
1:B:443:GLN:O	1:B:444:GLU:C	2.47	0.57
1:F:1516:LYS:CG	1:F:1517:ASN:H	2.12	0.57
1:F:1519:GLN:HE21	1:F:1519:GLN:N	1.95	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1581:VAL:N	1:F:1643:GLN:HE21	1.94	0.57
1:G:1804:PRO:HB3	1:G:1983:TRP:CZ2	2.39	0.57
1:C:660:THR:HG23	1:C:660:THR:O	2.04	0.57
1:F:1562:LEU:HD12	1:F:1568:ALA:CA	2.33	0.57
1:H:2131:THR:HA	1:H:2178:ILE:O	2.05	0.57
1:E:1283:TYR:CE1	1:E:1298:CYS:CB	2.88	0.57
1:G:1950:ARG:O	1:G:1951:LYS:C	2.45	0.57
1:D:960:THR:HA	1:D:999:ILE:O	2.03	0.57
1:B:410:HIS:CD2	1:B:436:ASN:HB3	2.40	0.57
1:E:1415:GLU:OE1	1:E:1417:TYR:OH	2.20	0.57
1:D:1109:ASN:CG	1:D:1110:LYS:H	2.13	0.57
1:F:1670:GLY:HA3	1:F:1718:LEU:CD2	2.35	0.57
1:G:1816:LYS:HG3	1:G:1817:ASN:N	2.19	0.57
1:B:321:ILE:HG22	1:B:460:TYR:CE1	2.39	0.57
1:E:1241:LEU:HG	1:E:1242:LEU:HG	1.87	0.57
1:F:1717:TYR:O	1:F:1718:LEU:HD23	2.04	0.57
1:E:1329:LEU:HD12	1:E:1329:LEU:C	2.30	0.56
1:A:4:PRO:HD3	1:A:183:TRP:NE1	2.19	0.56
1:D:983:TYR:CE1	1:D:998:CYS:HB3	2.40	0.56
1:H:2138:VAL:CG2	1:H:2139:ASP:H	2.16	0.56
1:A:23:PHE:HD1	1:A:23:PHE:H	1.53	0.56
1:A:82:GLU:HA	1:A:99:ILE:HG22	1.87	0.56
1:D:934:ASN:HB2	1:D:1006:HIS:CD2	2.40	0.56
1:D:1043:GLN:O	1:D:1044:GLU:C	2.49	0.56
1:E:1407:LEU:HD12	1:E:1407:LEU:O	2.05	0.56
1:H:2243:GLN:HG3	1:H:2301:TYR:CE1	2.40	0.56
1:B:377:ASP:OD1	1:B:406:HIS:HD2	1.88	0.56
1:E:1238:VAL:CG2	1:E:1239:ASP:N	2.68	0.56
1:E:1393:THR:O	1:E:1394:GLN:C	2.47	0.56
1:G:1976:PRO:HA	1:G:2012:SER:OG	2.05	0.56
1:C:642:LEU:O	1:C:644:HIS:N	2.39	0.56
1:C:683:TYR:CE1	1:C:698:CYS:HB2	2.40	0.56
1:D:1050:ARG:O	1:D:1051:LYS:C	2.48	0.56
1:F:1571:PHE:O	1:F:1572:LYS:C	2.47	0.56
1:A:59:LYS:HB2	1:A:89:LEU:CD2	2.33	0.56
1:C:777:LYS:HD3	1:C:777:LYS:C	2.31	0.56
1:D:1077:LYS:HB2	1:D:1111:THR:HB	1.87	0.56
1:A:127:GLN:O	1:A:127:GLN:HG2	2.06	0.56
1:C:704:THR:HG23	1:C:741:THR:HG22	1.88	0.56
1:C:770:GLY:O	1:C:786:PHE:HB2	2.06	0.56
1:F:1504:PRO:HB3	1:F:1683:TRP:CZ2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1582:GLU:HA	1:F:1599:ILE:HG22	1.88	0.56
1:A:81:VAL:H	1:A:143:GLN:HE21	1.52	0.56
1:A:110:HIS:CD2	1:A:136:ASN:HB3	2.41	0.56
1:E:1270:LEU:HD23	1:E:1270:LEU:O	2.06	0.56
1:E:1350:ARG:O	1:E:1354:ILE:HG13	2.05	0.56
1:F:1707:LEU:HD12	1:F:1707:LEU:C	2.31	0.56
1:G:1832:HIS:CE1	1:G:1850:VAL:HB	2.40	0.56
1:G:2017:TYR:O	1:G:2018:LEU:HD23	2.06	0.56
1:A:91:GLU:CB	1:C:691:GLU:HB3	2.26	0.56
1:C:724:ASP:OD2	1:C:819:THR:HA	2.06	0.56
1:E:1221:ILE:O	1:E:1224:LEU:HB2	2.06	0.56
1:E:1295:ARG:HB3	1:E:1295:ARG:HH11	1.68	0.56
1:F:1560:THR:HG23	1:F:1560:THR:O	2.05	0.56
1:H:2210:HIS:CD2	1:H:2236:ASN:HB3	2.41	0.56
1:H:2294:GLN:O	1:H:2295:SER:C	2.49	0.56
1:C:616:LYS:HG3	1:C:617:ASN:H	1.70	0.55
1:D:1120:THR:O	1:D:1121:LYS:C	2.49	0.55
1:F:1629:LEU:C	1:F:1629:LEU:HD12	2.31	0.55
1:A:217:TYR:O	1:A:218:LEU:HD23	2.06	0.55
1:B:356:ASP:N	1:B:395:ARG:HH12	2.04	0.55
1:C:796:LYS:HD3	1:C:797:TYR:N	2.20	0.55
1:E:1238:VAL:CG2	1:E:1239:ASP:H	2.18	0.55
1:E:1212:SER:HB3	1:E:1387:PHE:CE2	2.42	0.55
1:E:1216:LYS:HG3	1:E:1217:ASN:H	1.71	0.55
1:B:302:GLN:H	1:B:302:GLN:NE2	2.04	0.55
1:F:1647:TYR:O	1:F:1648:LYS:C	2.50	0.55
1:H:2162:LEU:HD12	1:H:2168:ALA:HA	1.88	0.55
1:C:679:TYR:CE2	1:C:744:GLU:HG3	2.42	0.55
1:F:1512:SER:OG	1:F:1668:GLU:HA	2.06	0.55
1:F:1623:ILE:O	1:F:1624:ASP:HB2	2.07	0.55
1:G:1910:HIS:NE2	1:G:1936:ASN:HB3	2.21	0.55
1:H:2239:MET:HE3	1:H:2306:THR:HG22	1.87	0.55
1:B:477:LYS:O	1:B:477:LYS:HD3	2.07	0.55
1:C:642:LEU:C	1:C:644:HIS:H	2.15	0.55
1:C:682:GLU:OE1	1:C:682:GLU:N	2.40	0.55
1:E:1274:LYS:HD2	1:E:1274:LYS:N	2.22	0.55
1:A:16:LYS:O	1:A:17:ASN:C	2.49	0.55
1:A:47:ILE:HD13	1:A:89:LEU:HD22	1.89	0.55
1:A:167:TYR:CD1	1:A:167:TYR:N	2.73	0.55
1:D:953:PRO:HG2	1:D:954:ASN:H	1.71	0.55
1:E:1367:TYR:CD1	1:E:1367:TYR:N	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1538:VAL:CG2	1:F:1539:ASP:N	2.69	0.55
1:G:1870:LEU:C	1:G:1870:LEU:HD23	2.31	0.55
1:B:331:THR:HG22	1:B:379:TYR:CD1	2.42	0.55
1:D:1067:TYR:N	1:D:1067:TYR:CD1	2.74	0.54
1:A:145:LEU:O	1:A:146:ASP:C	2.51	0.54
1:C:602:GLN:NE2	1:C:602:GLN:N	2.54	0.54
1:C:683:TYR:HB2	1:C:794:GLN:HE21	1.73	0.54
1:E:1240:GLN:HB2	1:E:1245:ASP:O	2.07	0.54
1:H:2195:ARG:HB3	1:H:2195:ARG:CZ	2.36	0.54
1:H:2279:LYS:HG3	1:H:2280:GLU:N	2.23	0.54
1:F:1523:PHE:HD1	1:F:1523:PHE:H	1.54	0.54
1:D:904:PRO:HD3	1:D:1083:TRP:NE1	2.23	0.54
1:E:1204:PRO:HB3	1:E:1383:TRP:CZ2	2.42	0.54
1:A:85:HIS:CD2	1:B:394:GLU:HG2	2.43	0.54
1:B:304:PRO:HD3	1:B:483:TRP:CE2	2.42	0.54
1:E:1379:LYS:HG3	1:E:1380:GLU:N	2.22	0.54
1:F:1651:LYS:HE2	1:F:1655:ASP:OD2	2.07	0.54
1:F:1667:TYR:N	1:F:1667:TYR:CD1	2.74	0.54
1:A:4:PRO:HB3	1:A:183:TRP:CZ2	2.42	0.54
1:A:129:LEU:C	1:A:129:LEU:HD12	2.31	0.54
1:F:1570:LEU:HD23	1:F:1570:LEU:C	2.33	0.54
1:D:916:LYS:HE2	1:D:1091:GLU:HA	1.89	0.54
1:D:1116:VAL:C	1:D:1117:TYR:CD1	2.86	0.54
1:E:1343:GLN:O	1:E:1344:GLU:C	2.51	0.54
1:E:1347:TYR:O	1:E:1348:LYS:C	2.49	0.54
1:F:1679:LYS:CG	1:F:1680:GLU:H	2.19	0.54
1:H:2138:VAL:CG2	1:H:2139:ASP:N	2.71	0.54
1:A:161:THR:O	1:A:163:GLY:N	2.41	0.54
1:C:631:THR:HG22	1:C:679:TYR:HD1	1.71	0.54
1:C:670:LEU:HD23	1:C:670:LEU:C	2.33	0.54
1:D:982:GLU:HA	1:D:999:ILE:HG22	1.90	0.54
1:F:1588:TYR:N	1:F:1588:TYR:CD1	2.76	0.54
1:F:1621:VAL:HG12	1:F:1622:SER:N	2.23	0.54
1:B:454:ILE:CG1	1:B:459:LEU:HB3	2.33	0.54
1:D:980:GLY:HA2	1:D:1043:GLN:NE2	2.22	0.54
1:E:1216:LYS:HE2	1:E:1391:GLU:HA	1.89	0.54
1:F:1531:THR:O	1:F:1532:HIS:CG	2.61	0.54
1:G:1840:GLN:O	1:G:1840:GLN:HG3	2.08	0.54
1:H:2142:LEU:O	1:H:2144:HIS:N	2.40	0.54
1:F:1562:LEU:CD1	1:F:1568:ALA:HA	2.37	0.54
1:E:1223:PHE:CE2	1:F:1595:ARG:CZ	2.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2104:PRO:HD3	1:H:2283:TRP:NE1	2.23	0.53
1:B:440:VAL:HG21	1:B:445:LEU:HD11	1.89	0.53
1:B:479:LYS:CG	1:B:480:GLU:H	2.05	0.53
1:D:977:ASP:OD1	1:D:1006:HIS:HD2	1.91	0.53
1:H:2195:ARG:NH1	1:H:2195:ARG:CB	2.69	0.53
1:A:98:CYS:O	1:A:99:ILE:HG23	2.09	0.53
1:A:179:LYS:CG	1:A:180:GLU:H	2.17	0.53
1:E:1262:LEU:CD2	1:E:1301:GLY:HA2	2.39	0.53
1:C:685:HIS:O	1:C:686:LEU:HB2	2.08	0.53
1:C:713:ILE:N	1:C:713:ILE:HD12	2.23	0.53
1:D:921:ILE:HG22	1:D:1060:TYR:CE1	2.44	0.53
1:E:1343:GLN:HG3	1:E:1401:TYR:CE1	2.44	0.53
1:G:1894:GLU:O	1:G:1895:ARG:HB2	2.08	0.53
1:H:2188:TYR:CD1	1:H:2188:TYR:N	2.76	0.53
1:H:2243:GLN:O	1:H:2244:GLU:C	2.50	0.53
1:A:115:LYS:HD3	1:A:210:LYS:HZ3	1.70	0.53
1:C:707:GLU:OE1	1:C:707:GLU:N	2.38	0.53
1:G:1879:TYR:CD2	1:G:1944:GLU:HG3	2.44	0.53
1:H:2115:VAL:CG1	1:H:2292:PHE:HE2	2.22	0.53
1:D:1107:LEU:O	1:D:1107:LEU:HD12	2.07	0.53
1:B:323:PHE:H	1:B:323:PHE:HD1	1.57	0.53
1:C:767:TYR:CD1	1:C:767:TYR:N	2.77	0.53
1:F:1654:ILE:CG1	1:F:1659:LEU:HB3	2.32	0.53
1:G:1824:LEU:HD13	1:G:1998:LEU:HD21	1.91	0.53
1:H:2110:HIS:ND1	1:H:2287:PHE:O	2.42	0.53
1:H:2209:ASN:O	1:H:2237:LYS:HA	2.09	0.53
1:B:382:GLU:CD	1:B:382:GLU:H	2.17	0.53
1:A:25:TYR:CZ	1:A:150:ARG:NH1	2.77	0.53
1:C:660:THR:HA	1:C:699:ILE:O	2.09	0.53
1:A:79:TYR:CD2	1:A:144:GLU:HA	2.44	0.52
1:A:87:CYS:SG	1:A:98:CYS:N	2.82	0.52
1:A:159:LEU:HG	1:A:160:TYR:CD2	2.44	0.52
1:C:619:GLN:O	1:C:622:TYR:HB3	2.09	0.52
1:C:694:GLU:O	1:C:695:ARG:HB2	2.09	0.52
1:D:1000:TYR:HE2	1:D:1099:MET:HG2	1.74	0.52
1:E:1309:ASN:O	1:E:1337:LYS:HA	2.09	0.52
1:F:1643:GLN:O	1:F:1644:GLU:C	2.51	0.52
1:G:1842:LEU:O	1:G:1844:HIS:N	2.42	0.52
1:H:2116:LYS:O	1:H:2118:LEU:N	2.42	0.52
1:B:447:TYR:O	1:B:448:LYS:C	2.52	0.52
1:A:98:CYS:O	1:A:99:ILE:CG2	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:PRO:HB3	1:B:483:TRP:CZ2	2.44	0.52
1:B:446:ASP:O	1:B:450:ARG:HG3	2.10	0.52
1:C:754:ILE:HA	1:C:759:LEU:H	1.74	0.52
1:D:917:ASN:HB3	1:D:919:GLN:OE1	2.08	0.52
1:D:1077:LYS:O	1:D:1077:LYS:HD3	2.08	0.52
1:E:1388:PRO:HG3	1:E:1392:PHE:CE2	2.44	0.52
1:F:1702:LYS:C	1:F:1704:ASN:H	2.15	0.52
1:G:1802:GLN:HE21	1:G:1802:GLN:N	2.07	0.52
1:H:2182:GLU:HA	1:H:2198:CYS:O	2.09	0.52
1:H:2279:LYS:HG3	1:H:2280:GLU:H	1.75	0.52
1:A:200:ILE:HG13	1:A:201:TYR:CD2	2.45	0.52
1:B:382:GLU:OE1	1:B:382:GLU:N	2.40	0.52
1:C:667:MET:O	1:C:670:LEU:HB3	2.10	0.52
1:D:942:LEU:C	1:D:944:HIS:H	2.18	0.52
1:A:70:LEU:O	1:A:70:LEU:HD23	2.09	0.52
1:D:1047:TYR:O	1:D:1050:ARG:N	2.43	0.52
1:E:1291:GLU:N	1:G:1891:GLU:OE1	2.28	0.52
1:G:1883:TYR:CE1	1:G:1898:CYS:HB2	2.44	0.52
1:G:1939:MET:HE3	1:G:2006:THR:HG22	1.90	0.52
1:H:2134:ASN:OD1	1:H:2175:ASN:HB3	2.10	0.52
1:E:1202:GLN:H	1:E:1202:GLN:NE2	2.08	0.52
1:G:1802:GLN:NE2	1:G:1802:GLN:N	2.56	0.52
1:G:1829:PRO:HD3	1:G:1947:TYR:OH	2.10	0.52
1:A:81:VAL:O	1:A:99:ILE:HG22	2.09	0.52
1:A:199:MET:C	1:A:201:TYR:H	2.16	0.52
1:C:743:GLN:OE1	1:C:801:TYR:HB3	2.09	0.52
1:D:994:GLU:O	1:D:995:ARG:HB2	2.09	0.52
1:E:1345:LEU:O	1:E:1346:ASP:C	2.53	0.52
1:F:1644:GLU:O	1:F:1645:LEU:C	2.52	0.52
1:H:2115:VAL:O	1:H:2116:LYS:O	2.27	0.52
1:A:56:ASP:N	1:A:95:ARG:HH12	2.07	0.52
1:B:509:ASN:CG	1:B:510:LYS:H	2.17	0.52
1:C:670:LEU:O	1:C:674:LYS:HD3	2.09	0.52
1:H:2129:PRO:HD3	1:H:2247:TYR:CZ	2.44	0.52
1:H:2142:LEU:C	1:H:2144:HIS:N	2.66	0.52
1:B:412:GLU:HB3	1:B:413:ILE:HD12	1.92	0.52
1:C:615:VAL:HG11	1:C:618:LEU:HD13	1.92	0.52
1:D:1007:GLU:OE1	1:D:1007:GLU:N	2.43	0.52
1:E:1247:ILE:HD13	1:E:1289:LEU:HD22	1.92	0.52
1:F:1583:TYR:CE2	1:F:1695:SER:HB3	2.45	0.52
1:F:1585:HIS:O	1:F:1586:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1959:LEU:HG	1:G:1960:TYR:CD2	2.45	0.52
1:H:2195:ARG:CB	1:H:2195:ARG:HH11	2.23	0.52
1:A:2:GLN:HE21	1:A:2:GLN:N	2.07	0.52
1:D:938:VAL:HG23	1:D:939:ASP:N	2.24	0.52
1:D:982:GLU:OE1	1:D:982:GLU:N	2.43	0.52
1:A:85:HIS:O	1:A:86:LEU:HB2	2.10	0.51
1:A:143:GLN:HG3	1:A:201:TYR:CE1	2.45	0.51
1:E:1312:GLU:C	1:E:1313:ILE:HD12	2.35	0.51
1:G:1830:VAL:HG21	1:G:1882:GLU:HB3	1.92	0.51
1:G:1907:GLU:OE1	1:G:1907:GLU:N	2.43	0.51
1:C:729:LEU:HD12	1:C:729:LEU:C	2.35	0.51
1:B:404:THR:CG2	1:B:441:THR:HG22	2.40	0.51
1:F:1559:LYS:HB2	1:F:1589:LEU:CD2	2.36	0.51
1:G:1935:THR:OG1	1:G:1936:ASN:N	2.40	0.51
1:B:304:PRO:HD3	1:B:483:TRP:NE1	2.24	0.51
1:C:740:VAL:HG21	1:C:745:LEU:HD11	1.93	0.51
1:D:930:VAL:HG13	1:D:955:TYR:OH	2.10	0.51
1:D:1058:GLN:N	1:D:1058:GLN:CD	2.68	0.51
1:F:1604:THR:HG23	1:F:1641:THR:HG22	1.93	0.51
1:C:645:ASP:O	1:C:646:LEU:HD23	2.10	0.51
1:E:1354:ILE:HA	1:E:1359:LEU:H	1.75	0.51
1:E:1402:LYS:C	1:E:1404:ASN:N	2.68	0.51
1:A:113:ILE:N	1:A:113:ILE:HD12	2.25	0.51
1:A:119:VAL:HG22	1:A:214:ILE:HB	1.93	0.51
1:C:779:LYS:HG3	1:C:780:GLU:N	2.26	0.51
1:F:1502:GLN:H	1:F:1502:GLN:NE2	2.09	0.51
1:F:1615:LYS:HG2	1:F:1709:ASN:HD22	1.75	0.51
1:H:2156:ASP:N	1:H:2195:ARG:HH12	2.09	0.51
1:H:2177:ASP:OD2	1:H:2206:HIS:HA	2.11	0.51
1:A:10:HIS:CD2	1:A:10:HIS:N	2.79	0.51
1:A:67:MET:O	1:A:70:LEU:HB3	2.11	0.51
1:D:983:TYR:CE1	1:D:998:CYS:HB2	2.45	0.51
1:D:988:TYR:N	1:D:988:TYR:CD1	2.79	0.51
1:A:70:LEU:HD23	1:A:70:LEU:C	2.35	0.51
1:B:380:GLY:HA2	1:B:443:GLN:HE21	1.76	0.51
1:F:1540:GLN:HB2	1:F:1545:ASP:O	2.11	0.51
1:G:1877:ASP:OD1	1:G:1906:HIS:CD2	2.64	0.51
1:G:1954:ILE:HG12	1:G:1959:LEU:HB3	1.91	0.51
1:D:1004:THR:HG23	1:D:1041:THR:HG22	1.93	0.51
1:F:1579:TYR:CD2	1:F:1644:GLU:HG3	2.46	0.51
1:H:2296:LYS:HD3	1:H:2297:TYR:CA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1943:GLN:O	1:G:1944:GLU:C	2.54	0.50
1:A:145:LEU:O	1:A:147:TYR:N	2.45	0.50
1:B:445:LEU:O	1:B:446:ASP:C	2.54	0.50
1:E:1285:HIS:O	1:E:1286:LEU:HB2	2.11	0.50
1:G:1996:LYS:HD3	1:G:1997:TYR:CA	2.41	0.50
1:C:635:VAL:O	1:C:675:ASN:HA	2.10	0.50
1:D:902:GLN:NE2	1:D:902:GLN:H	2.10	0.50
1:E:1260:THR:HG23	1:E:1260:THR:O	2.11	0.50
1:F:1670:GLY:CA	1:F:1718:LEU:HD23	2.40	0.50
1:G:1912:GLU:C	1:G:1913:ILE:HD12	2.37	0.50
1:G:1950:ARG:O	1:G:1954:ILE:HG13	2.09	0.50
1:H:2125:TYR:CD2	1:H:2250:ARG:HD2	2.46	0.50
1:H:2250:ARG:O	1:H:2251:LYS:C	2.53	0.50
1:A:30:VAL:CG2	1:A:82:GLU:HB3	2.40	0.50
1:C:685:HIS:O	1:C:686:LEU:CB	2.60	0.50
1:D:982:GLU:HA	1:D:998:CYS:O	2.12	0.50
1:D:983:TYR:CE1	1:D:1000:TYR:HE1	2.29	0.50
1:F:1530:VAL:HG21	1:F:1582:GLU:HB3	1.93	0.50
1:A:79:TYR:CE2	1:A:144:GLU:HA	2.47	0.50
1:A:196:LYS:HD3	1:A:197:TYR:CA	2.41	0.50
1:C:709:ASN:O	1:C:737:LYS:HA	2.11	0.50
1:C:744:GLU:O	1:C:747:TYR:HB3	2.12	0.50
1:C:783:TRP:O	1:C:784:PHE:HD2	1.95	0.50
1:E:1327:GLN:O	1:E:1327:GLN:HG2	2.12	0.50
1:F:1720:THR:HG22	1:F:1720:THR:O	2.10	0.50
1:G:1819:GLN:O	1:G:1822:TYR:HB3	2.12	0.50
1:G:1823:PHE:H	1:G:1823:PHE:HD1	1.59	0.50
1:A:16:LYS:HD3	1:A:191:GLU:HG2	1.93	0.50
1:B:341:LEU:HG	1:B:342:LEU:HG	1.92	0.50
1:B:379:TYR:CD2	1:B:444:GLU:HG3	2.47	0.50
1:B:385:HIS:O	1:B:386:LEU:HB2	2.11	0.50
1:B:404:THR:HG23	1:B:441:THR:HG22	1.94	0.50
1:D:1077:LYS:CB	1:D:1111:THR:HB	2.41	0.50
1:B:459:LEU:HG	1:B:460:TYR:CD2	2.46	0.50
1:A:19:GLN:O	1:A:22:TYR:HB3	2.12	0.50
1:D:1077:LYS:HD3	1:D:1077:LYS:C	2.37	0.50
1:F:1530:VAL:HG13	1:F:1555:TYR:OH	2.11	0.50
1:B:343:SER:HB2	1:C:789:GLU:HB3	1.94	0.50
1:B:355:TYR:C	1:B:395:ARG:HH12	2.20	0.50
1:B:374:LYS:HD2	1:B:374:LYS:N	2.26	0.50
1:G:1877:ASP:OD1	1:G:1906:HIS:HD2	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2182:GLU:HA	1:H:2199:ILE:HG22	1.93	0.50
1:C:776:PRO:HB2	1:C:779:LYS:HB3	1.94	0.49
1:C:782:PHE:CE2	1:C:805:GLU:HG2	2.47	0.49
1:G:2003:ASP:O	1:G:2004:ASN:C	2.55	0.49
1:D:994:GLU:O	1:D:995:ARG:CB	2.60	0.49
1:D:1050:ARG:O	1:D:1054:ILE:HG13	2.12	0.49
1:E:1359:LEU:HG	1:E:1360:TYR:CE2	2.47	0.49
1:A:115:LYS:HE3	1:A:210:LYS:HD3	1.93	0.49
1:D:1013:ILE:HD12	1:D:1013:ILE:N	2.27	0.49
1:E:1291:GLU:OE2	1:G:1890:CYS:HA	2.12	0.49
1:F:1585:HIS:C	1:F:1586:LEU:HG	2.38	0.49
1:H:2177:ASP:OD1	1:H:2206:HIS:CD2	2.66	0.49
1:A:16:LYS:HG3	1:A:17:ASN:N	2.28	0.49
1:A:143:GLN:OE1	1:A:201:TYR:HB3	2.13	0.49
1:A:146:ASP:O	1:A:150:ARG:HG3	2.12	0.49
1:C:695:ARG:HB3	1:C:695:ARG:NH1	2.28	0.49
1:E:1231:THR:HG22	1:E:1279:TYR:CD1	2.47	0.49
1:F:1502:GLN:H	1:F:1502:GLN:HE21	1.60	0.49
1:H:2145:ASP:C	1:H:2145:ASP:OD1	2.55	0.49
1:H:2245:LEU:O	1:H:2246:ASP:C	2.55	0.49
1:B:319:GLN:O	1:B:322:TYR:N	2.45	0.49
1:C:760:TYR:OH	1:C:786:PHE:O	2.28	0.49
1:E:1407:LEU:HD12	1:E:1407:LEU:C	2.36	0.49
1:F:1702:LYS:C	1:F:1704:ASN:N	2.69	0.49
1:B:382:GLU:HA	1:B:399:ILE:HG22	1.94	0.49
1:C:621:ILE:O	1:C:624:LEU:HB2	2.13	0.49
1:C:642:LEU:C	1:C:644:HIS:N	2.71	0.49
1:D:1045:LEU:HD12	1:D:1074:PHE:HE2	1.78	0.49
1:E:1242:LEU:C	1:E:1244:HIS:H	2.20	0.49
1:F:1651:LYS:O	1:F:1654:ILE:HB	2.11	0.49
1:H:2150:VAL:HG23	1:H:2155:TYR:HE1	1.77	0.49
1:A:172:ILE:HB	1:A:186:PHE:CE2	2.46	0.49
1:D:1043:GLN:OE1	1:D:1101:TYR:HB3	2.12	0.49
1:F:1672:ILE:HB	1:F:1686:PHE:CE2	2.47	0.49
1:H:2129:PRO:HD3	1:H:2247:TYR:CE2	2.48	0.49
1:H:2183:TYR:CE2	1:H:2295:SER:HB3	2.48	0.49
1:H:2259:LEU:O	1:H:2265:SER:OG	2.30	0.49
1:C:630:VAL:CG2	1:C:682:GLU:HB3	2.43	0.49
1:C:688:TYR:CD1	1:C:688:TYR:N	2.80	0.49
1:E:1391:GLU:N	1:H:2143:SER:OG	2.45	0.49
1:H:2200:TYR:CE2	1:H:2299:MET:HG2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLN:HE21	1:B:302:GLN:N	2.11	0.49
1:C:643:SER:O	1:C:665:GLN:HA	2.13	0.49
1:D:945:ASP:OD1	1:D:945:ASP:C	2.56	0.49
1:E:1255:TYR:C	1:E:1295:ARG:HH12	2.21	0.49
1:E:1402:LYS:C	1:E:1404:ASN:H	2.21	0.49
1:G:1817:ASN:HA	1:G:1819:GLN:HE22	1.77	0.49
1:G:2020:THR:O	1:G:2021:LYS:C	2.55	0.49
1:H:2194:GLU:O	1:H:2195:ARG:HB2	2.13	0.49
1:D:987:CYS:SG	1:D:997:ALA:C	2.96	0.49
1:G:1888:TYR:CD1	1:G:1888:TYR:N	2.80	0.49
1:H:2180:GLY:CA	1:H:2243:GLN:NE2	2.76	0.49
1:D:940:GLN:HB2	1:D:945:ASP:O	2.13	0.48
1:D:942:LEU:C	1:D:944:HIS:N	2.71	0.48
1:D:970:LEU:HD23	1:D:970:LEU:C	2.38	0.48
1:A:192:PHE:CD1	1:A:192:PHE:C	2.90	0.48
1:B:368:ALA:O	1:B:369:THR:C	2.57	0.48
1:B:391:GLU:CD	1:D:991:GLU:H	2.20	0.48
1:B:413:ILE:HD12	1:B:413:ILE:N	2.28	0.48
1:B:499:MET:C	1:B:501:TYR:N	2.71	0.48
1:C:735:THR:OG1	1:C:736:ASN:N	2.46	0.48
1:C:750:ARG:O	1:C:751:LYS:C	2.55	0.48
1:F:1525:TYR:CZ	1:F:1650:ARG:NH1	2.81	0.48
1:G:1941:THR:C	1:G:1943:GLN:N	2.68	0.48
1:H:2115:VAL:HG11	1:H:2118:LEU:HD13	1.95	0.48
1:H:2170:LEU:HD22	1:H:2171:PHE:CD1	2.48	0.48
1:A:87:CYS:SG	1:A:97:ALA:C	2.96	0.48
1:C:743:GLN:HG3	1:C:801:TYR:CE1	2.48	0.48
1:D:1100:ILE:HG13	1:D:1101:TYR:CD2	2.48	0.48
1:F:1591:GLU:OE1	1:H:2191:GLU:HG2	2.13	0.48
1:G:1862:LEU:HD13	1:G:1867:MET:HG2	1.95	0.48
1:G:1879:TYR:CE2	1:G:1944:GLU:HA	2.48	0.48
1:E:1260:THR:HA	1:E:1299:ILE:O	2.13	0.48
1:D:923:PHE:HD1	1:D:923:PHE:H	1.62	0.48
1:D:1029:LEU:C	1:D:1029:LEU:CD1	2.86	0.48
1:D:1096:LYS:HD3	1:D:1097:TYR:N	2.28	0.48
1:G:1993:THR:HA	1:H:2194:GLU:OE2	2.13	0.48
1:H:2117:ASN:HB3	1:H:2119:GLN:OE1	2.13	0.48
1:H:2320:THR:O	1:H:2320:THR:HG22	2.13	0.48
1:C:716:LYS:HG2	1:C:734:GLU:HG2	1.95	0.48
1:D:1000:TYR:O	1:D:1001:GLY:C	2.57	0.48
1:D:1092:PHE:CD1	1:D:1092:PHE:C	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1589:LEU:HD12	1:F:1596:SER:HB3	1.95	0.48
1:H:2168:ALA:C	1:H:2170:LEU:H	2.22	0.48
1:A:32:HIS:CE1	1:A:50:VAL:HB	2.49	0.48
1:A:67:MET:O	1:A:68:ALA:C	2.57	0.48
1:C:634:ASN:OD1	1:C:675:ASN:HB3	2.13	0.48
1:C:685:HIS:CD2	1:C:686:LEU:HG	2.49	0.48
1:D:916:LYS:CG	1:D:917:ASN:H	2.20	0.48
1:D:1023:ILE:O	1:D:1024:ASP:HB2	2.14	0.48
1:F:1531:THR:HG22	1:F:1579:TYR:CD1	2.49	0.48
1:F:1645:LEU:O	1:F:1646:ASP:C	2.56	0.48
1:F:1674:PHE:HB2	1:F:1682:PHE:CE1	2.49	0.48
1:H:2145:ASP:CG	1:H:2159:LYS:HD2	2.38	0.48
1:B:496:LYS:HD3	1:B:496:LYS:O	2.13	0.48
1:D:919:GLN:C	1:D:921:ILE:H	2.21	0.48
1:B:383:TYR:CZ	1:B:398:CYS:HB2	2.48	0.48
1:E:1270:LEU:HD23	1:E:1270:LEU:C	2.38	0.48
1:F:1585:HIS:O	1:F:1586:LEU:CB	2.61	0.48
1:H:2170:LEU:HD23	1:H:2170:LEU:C	2.39	0.48
1:A:194:GLN:O	1:A:195:SER:C	2.57	0.48
1:B:443:GLN:HG3	1:B:501:TYR:CD1	2.49	0.48
1:B:507:LEU:HD12	1:B:507:LEU:C	2.38	0.48
1:G:1840:GLN:HB2	1:G:1845:ASP:O	2.13	0.48
1:A:121:VAL:O	1:A:127:GLN:HA	2.14	0.47
1:B:315:VAL:HG13	1:B:492:PHE:HE2	1.78	0.47
1:D:1074:PHE:HB2	1:D:1082:PHE:CE1	2.49	0.47
1:F:1502:GLN:HE21	1:F:1502:GLN:N	2.12	0.47
1:F:1510:HIS:N	1:F:1510:HIS:CD2	2.81	0.47
1:H:2177:ASP:OD1	1:H:2206:HIS:HD2	1.97	0.47
1:H:2297:TYR:C	1:H:2299:MET:H	2.20	0.47
1:E:1313:ILE:HD12	1:E:1313:ILE:N	2.29	0.47
1:H:2254:ILE:O	1:H:2258:GLN:HA	2.14	0.47
1:A:56:ASP:O	1:A:57:LYS:HD3	2.14	0.47
1:A:112:GLU:C	1:A:113:ILE:HD12	2.39	0.47
1:B:499:MET:C	1:B:501:TYR:H	2.22	0.47
1:F:1600:TYR:CE2	1:F:1699:MET:HG2	2.49	0.47
1:F:1658:GLN:N	1:F:1658:GLN:CD	2.72	0.47
1:C:741:THR:O	1:C:742:ALA:C	2.56	0.47
1:D:1108:ASP:OD2	1:D:1111:THR:HG23	2.14	0.47
1:E:1324:ASP:OD2	1:E:1419:THR:HA	2.14	0.47
1:C:732:ASP:O	1:C:733:ILE:HG23	2.14	0.47
1:D:1038:LYS:O	1:D:1109:ASN:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1059:LEU:O	1:D:1065:SER:OG	2.29	0.47
1:C:655:TYR:CD1	1:C:655:TYR:C	2.92	0.47
1:H:2117:ASN:HA	1:H:2119:GLN:HE22	1.79	0.47
1:A:19:GLN:HG2	1:A:20:ASN:N	2.29	0.47
1:A:25:TYR:CD2	1:A:150:ARG:HD2	2.50	0.47
1:B:332:HIS:CD2	1:B:350:VAL:HG21	2.50	0.47
1:E:1337:LYS:HB2	1:E:1340:VAL:HG12	1.96	0.47
1:E:1343:GLN:OE1	1:E:1401:TYR:HB3	2.13	0.47
1:F:1640:VAL:HG21	1:F:1645:LEU:HD11	1.97	0.47
1:G:1831:THR:HG22	1:G:1879:TYR:CD1	2.50	0.47
1:C:623:PHE:HD1	1:C:623:PHE:H	1.63	0.47
1:G:1946:ASP:OD2	1:G:1950:ARG:NE	2.48	0.47
1:H:2131:THR:HG22	1:H:2179:TYR:CE1	2.50	0.47
1:H:2246:ASP:O	1:H:2250:ARG:HG3	2.14	0.47
1:H:2267:TYR:HD1	1:H:2267:TYR:H	1.62	0.47
1:B:496:LYS:C	1:B:496:LYS:CD	2.83	0.47
1:D:919:GLN:NE2	1:D:919:GLN:N	2.50	0.47
1:F:1518:LEU:O	1:F:1519:GLN:C	2.56	0.47
1:F:1654:ILE:HA	1:F:1659:LEU:H	1.80	0.47
1:G:1909:ASN:O	1:G:1937:LYS:HA	2.14	0.47
1:A:95:ARG:NE	1:B:323:PHE:CE2	2.83	0.47
1:A:170:GLY:O	1:A:186:PHE:HB2	2.15	0.47
1:A:196:LYS:HD3	1:A:197:TYR:HA	1.96	0.47
1:B:358:LEU:HD12	1:B:397:ALA:O	2.14	0.47
1:B:467:TYR:CD2	1:B:518:LEU:HB3	2.50	0.47
1:E:1216:LYS:O	1:E:1218:LEU:N	2.48	0.47
1:F:1512:SER:HG	1:F:1668:GLU:HA	1.78	0.47
1:G:1874:LYS:HD2	1:G:1874:LYS:N	2.29	0.47
1:H:2150:VAL:HG23	1:H:2155:TYR:CE1	2.50	0.47
1:H:2183:TYR:CE1	1:H:2198:CYS:HB2	2.50	0.47
1:H:2272:ILE:HG22	1:H:2284:PHE:HB2	1.98	0.47
1:A:143:GLN:HG3	1:A:201:TYR:CD1	2.51	0.46
1:B:385:HIS:CD2	1:B:386:LEU:HG	2.49	0.46
1:C:759:LEU:HG	1:C:760:TYR:CD2	2.50	0.46
1:D:919:GLN:O	1:D:922:TYR:HB3	2.15	0.46
1:G:1972:ILE:HG12	1:G:1974:PHE:CE1	2.51	0.46
1:H:2155:TYR:O	1:H:2155:TYR:CD1	2.68	0.46
1:B:325:TYR:CZ	1:B:450:ARG:NH1	2.83	0.46
1:H:2160:THR:HA	1:H:2199:ILE:O	2.14	0.46
1:D:990:CYS:C	1:D:992:ASN:N	2.71	0.46
1:E:1295:ARG:HH11	1:E:1295:ARG:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1304:THR:CG2	1:E:1341:THR:HG22	2.45	0.46
1:F:1659:LEU:HG	1:F:1660:TYR:CD2	2.50	0.46
1:G:1885:HIS:O	1:G:1886:LEU:HB2	2.15	0.46
1:H:2104:PRO:HB3	1:H:2283:TRP:CZ2	2.50	0.46
1:B:429:LEU:C	1:B:429:LEU:CD1	2.89	0.46
1:E:1242:LEU:C	1:E:1244:HIS:N	2.74	0.46
1:F:1540:GLN:HG3	1:F:1540:GLN:O	2.14	0.46
1:G:1885:HIS:O	1:G:1886:LEU:CB	2.64	0.46
1:G:2000:ILE:HG13	1:G:2001:TYR:CD2	2.51	0.46
1:A:199:MET:C	1:A:201:TYR:N	2.74	0.46
1:H:2213:ILE:N	1:H:2213:ILE:HD12	2.31	0.46
1:B:394:GLU:O	1:B:395:ARG:HB2	2.15	0.46
1:B:419:VAL:HG22	1:B:514:ILE:HB	1.98	0.46
1:E:1323:ILE:O	1:E:1324:ASP:HB2	2.16	0.46
1:G:1852:GLY:HA3	1:G:1855:TYR:CZ	2.51	0.46
1:G:1972:ILE:HB	1:G:1986:PHE:CE2	2.51	0.46
1:B:319:GLN:O	1:B:322:TYR:HB3	2.16	0.46
1:C:802:LYS:C	1:C:804:ASN:N	2.74	0.46
1:E:1216:LYS:CG	1:E:1217:ASN:H	2.26	0.46
1:G:1816:LYS:O	1:G:1818:LEU:N	2.49	0.46
1:G:1917:ILE:O	1:G:1932:ASP:HA	2.16	0.46
1:H:2211:LEU:HD23	1:H:2238:LYS:HE2	1.97	0.46
1:H:2252:TYR:O	1:H:2254:ILE:N	2.49	0.46
1:A:140:VAL:HG21	1:A:145:LEU:HD11	1.97	0.46
1:D:970:LEU:O	1:D:974:LYS:HD3	2.15	0.46
1:E:1247:ILE:HD13	1:E:1289:LEU:CD2	2.46	0.46
1:E:1321:VAL:HG12	1:E:1322:SER:N	2.31	0.46
1:G:1879:TYR:CD2	1:G:1944:GLU:HA	2.51	0.46
1:H:2168:ALA:C	1:H:2170:LEU:N	2.72	0.46
1:A:117:ILE:HD11	1:A:209:ASN:HB2	1.97	0.46
1:E:1390:PRO:HD3	1:H:2165:GLN:OE1	2.15	0.46
1:F:1516:LYS:HE2	1:F:1692:PHE:H	1.81	0.46
1:H:2167:MET:O	1:H:2170:LEU:HB3	2.16	0.46
1:A:124:ASP:OD2	1:A:219:THR:HA	2.16	0.45
1:C:623:PHE:CE2	1:D:995:ARG:NH2	2.84	0.45
1:C:677:ASP:OD1	1:C:706:HIS:CD2	2.66	0.45
1:C:783:TRP:O	1:C:784:PHE:CD2	2.69	0.45
1:D:1010:HIS:CD2	1:D:1036:ASN:HB3	2.51	0.45
1:E:1252:GLY:HA3	1:E:1255:TYR:CE2	2.51	0.45
1:G:1804:PRO:HA	1:G:1808:GLN:NE2	2.31	0.45
1:G:1879:TYR:HH	1:G:1947:TYR:HD2	1.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2105:ASP:C	1:H:2107:SER:H	2.23	0.45
1:H:2146:LEU:O	1:H:2159:LYS:HA	2.16	0.45
1:H:2277:LYS:CB	1:H:2311:THR:HB	2.46	0.45
1:H:2314:ILE:HG22	1:H:2315:GLU:N	2.31	0.45
1:A:80:GLY:HA2	1:A:143:GLN:NE2	2.32	0.45
1:A:88:TYR:CD1	1:A:88:TYR:N	2.84	0.45
1:A:220:THR:O	1:A:221:LYS:C	2.58	0.45
1:B:388:TYR:N	1:B:388:TYR:CD1	2.83	0.45
1:B:467:TYR:N	1:B:467:TYR:CD1	2.85	0.45
1:C:679:TYR:CD2	1:C:744:GLU:HA	2.51	0.45
1:E:1217:ASN:CA	1:E:1219:GLN:HE22	2.29	0.45
1:E:1259:LYS:HG2	1:E:1260:THR:N	2.31	0.45
1:E:1402:LYS:O	1:E:1404:ASN:N	2.49	0.45
1:F:1643:GLN:HG3	1:F:1701:TYR:CD1	2.51	0.45
1:G:1900:TYR:CE2	1:G:1999:MET:HG2	2.51	0.45
1:G:1941:THR:O	1:G:1942:ALA:C	2.59	0.45
1:H:2123:PHE:HD1	1:H:2123:PHE:H	1.64	0.45
1:H:2183:TYR:CE1	1:H:2198:CYS:CB	3.00	0.45
1:A:144:GLU:O	1:A:147:TYR:HB3	2.16	0.45
1:F:1614:PRO:HB3	1:F:1634:GLU:HB3	1.98	0.45
1:G:1810:HIS:ND1	1:G:1987:PHE:O	2.50	0.45
1:G:1932:ASP:OD2	1:G:1932:ASP:N	2.50	0.45
1:H:2104:PRO:HD3	1:H:2283:TRP:CD1	2.51	0.45
1:B:459:LEU:HG	1:B:460:TYR:CE2	2.51	0.45
1:F:1541:LEU:HG	1:F:1542:LEU:N	2.32	0.45
1:H:2252:TYR:C	1:H:2254:ILE:N	2.73	0.45
1:H:2254:ILE:CG1	1:H:2259:LEU:HB3	2.31	0.45
1:A:77:ASP:OD1	1:A:106:HIS:CD2	2.68	0.45
1:B:318:LEU:O	1:B:319:GLN:C	2.59	0.45
1:B:370:LEU:HD23	1:B:370:LEU:C	2.42	0.45
1:C:677:ASP:OD2	1:C:706:HIS:HA	2.16	0.45
1:E:1394:GLN:O	1:E:1395:SER:C	2.59	0.45
1:H:2185:HIS:O	1:H:2186:LEU:HB2	2.17	0.45
1:H:2229:LEU:HD12	1:H:2229:LEU:C	2.42	0.45
1:H:2292:PHE:CD1	1:H:2292:PHE:C	2.94	0.45
1:A:12:SER:O	1:A:13:SER:C	2.57	0.45
1:A:74:LYS:HD2	1:A:74:LYS:N	2.32	0.45
1:A:151:LYS:HE2	1:A:155:ASP:OD2	2.16	0.45
1:B:380:GLY:CA	1:B:443:GLN:NE2	2.79	0.45
1:F:1524:LEU:HD11	1:F:1694:GLN:HG2	1.99	0.45
1:G:1843:SER:HB3	1:G:1865:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1904:THR:HG23	1:G:1941:THR:HG22	1.99	0.45
1:G:1976:PRO:HD2	1:G:1980:GLU:O	2.16	0.45
1:A:15:VAL:HG12	1:A:16:LYS:O	2.17	0.45
1:B:305:ASP:O	1:B:307:SER:N	2.49	0.45
1:C:747:TYR:O	1:C:748:LYS:C	2.60	0.45
1:F:1646:ASP:O	1:F:1650:ARG:HG3	2.16	0.45
1:H:2183:TYR:CE1	1:H:2200:TYR:HE1	2.35	0.45
1:H:2215:LYS:HE3	1:H:2310:LYS:HD3	1.98	0.45
1:H:2307:LEU:HD12	1:H:2307:LEU:C	2.41	0.45
1:B:441:THR:O	1:B:442:ALA:C	2.58	0.45
1:C:694:GLU:O	1:C:695:ARG:CB	2.65	0.45
1:C:802:LYS:C	1:C:804:ASN:H	2.24	0.45
1:E:1256:ASP:O	1:E:1257:LYS:HD3	2.17	0.45
1:G:1815:VAL:HG13	1:G:1992:PHE:HE2	1.80	0.45
1:G:1859:LYS:HB2	1:G:1889:LEU:CD2	2.40	0.45
1:B:440:VAL:CG2	1:B:445:LEU:HD11	2.47	0.45
1:C:694:GLU:HG2	1:D:985:HIS:CD2	2.51	0.45
1:D:938:VAL:CG2	1:D:939:ASP:N	2.79	0.45
1:D:956:ASP:O	1:D:957:LYS:CD	2.64	0.45
1:C:659:LYS:HG2	1:C:660:THR:N	2.32	0.45
1:D:910:HIS:N	1:D:910:HIS:CD2	2.84	0.45
1:D:919:GLN:C	1:D:921:ILE:N	2.74	0.45
1:D:1059:LEU:HG	1:D:1060:TYR:CD2	2.52	0.45
1:E:1294:GLU:O	1:E:1295:ARG:HB2	2.17	0.45
1:G:1913:ILE:HA	1:G:1914:PRO:HD3	1.86	0.45
1:H:2166:GLU:O	1:H:2167:MET:C	2.60	0.45
1:A:19:GLN:O	1:A:22:TYR:N	2.51	0.44
1:B:415:LYS:HG2	1:B:509:ASN:HD22	1.82	0.44
1:F:1583:TYR:HB2	1:F:1694:GLN:NE2	2.32	0.44
1:F:1624:ASP:OD2	1:F:1719:THR:HA	2.16	0.44
1:H:2185:HIS:CD2	1:H:2186:LEU:HG	2.51	0.44
1:A:52:GLY:HA3	1:A:55:TYR:CZ	2.52	0.44
1:A:98:CYS:C	1:A:99:ILE:HG23	2.42	0.44
1:B:454:ILE:HG12	1:B:460:TYR:H	1.81	0.44
1:C:623:PHE:CE2	1:D:995:ARG:CZ	3.01	0.44
1:C:772:ILE:HB	1:C:786:PHE:CZ	2.53	0.44
1:E:1309:ASN:O	1:E:1309:ASN:CG	2.59	0.44
1:F:1697:TYR:O	1:F:1700:ILE:HG23	2.17	0.44
1:H:2143:SER:O	1:H:2165:GLN:HA	2.16	0.44
1:A:15:VAL:HA	1:A:190:PRO:HA	1.97	0.44
1:B:310:HIS:N	1:B:310:HIS:CD2	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:777:LYS:HB2	1:C:811:THR:HB	2.00	0.44
1:D:919:GLN:HE21	1:D:919:GLN:N	2.05	0.44
1:D:904:PRO:HB3	1:D:1083:TRP:CH2	2.52	0.44
1:D:946:LEU:O	1:D:959:LYS:HA	2.18	0.44
1:D:1000:TYR:N	1:D:1000:TYR:CD1	2.85	0.44
1:A:85:HIS:CD2	1:A:86:LEU:HG	2.52	0.44
1:A:147:TYR:O	1:A:148:LYS:C	2.61	0.44
1:B:427:GLN:O	1:B:427:GLN:HG2	2.16	0.44
1:D:1066:LYS:HB3	1:D:1067:TYR:CE1	2.53	0.44
1:D:1067:TYR:CD2	1:D:1118:LEU:HD13	2.52	0.44
1:E:1317:ILE:HD11	1:E:1409:ASN:HB2	1.99	0.44
1:F:1567:MET:O	1:F:1570:LEU:HB3	2.17	0.44
1:G:1870:LEU:O	1:G:1870:LEU:HD23	2.17	0.44
1:G:1895:ARG:NH1	1:G:1895:ARG:HB3	2.33	0.44
1:G:1923:ILE:O	1:G:1926:ILE:HG12	2.17	0.44
1:A:16:LYS:HE2	1:A:192:PHE:N	2.28	0.44
1:B:334:ASN:HB2	1:B:406:HIS:NE2	2.32	0.44
1:D:929:PRO:HD3	1:D:1047:TYR:OH	2.17	0.44
1:F:1547:ILE:HD13	1:F:1589:LEU:CD2	2.45	0.44
1:F:1594:GLU:O	1:F:1595:ARG:CB	2.66	0.44
1:G:1966:LYS:HB3	1:G:1967:TYR:CD1	2.53	0.44
1:H:2297:TYR:O	1:H:2299:MET:N	2.51	0.44
1:A:58:LEU:HD12	1:A:97:ALA:O	2.17	0.44
1:D:929:PRO:HD3	1:D:1047:TYR:CE2	2.52	0.44
1:D:1047:TYR:O	1:D:1048:LYS:C	2.60	0.44
1:D:1072:ILE:HB	1:D:1086:PHE:CZ	2.53	0.44
1:C:601:GLN:OE1	1:C:783:TRP:NE1	2.51	0.44
1:D:1102:LYS:C	1:D:1104:ASN:N	2.74	0.44
1:E:1219:GLN:O	1:E:1222:TYR:HB3	2.18	0.44
1:G:1883:TYR:CE1	1:G:1900:TYR:HE1	2.35	0.44
1:H:2105:ASP:O	1:H:2107:SER:N	2.50	0.44
1:H:2221:VAL:HB	1:H:2229:LEU:CD1	2.46	0.44
1:B:334:ASN:OD1	1:B:375:ASN:HB3	2.18	0.44
1:C:674:LYS:N	1:C:674:LYS:CD	2.81	0.44
1:C:709:ASN:O	1:C:709:ASN:CG	2.60	0.44
1:D:912:SER:HB3	1:D:1087:PHE:CE2	2.53	0.44
1:D:1054:ILE:HA	1:D:1059:LEU:H	1.82	0.44
1:E:1210:HIS:CD2	1:E:1210:HIS:N	2.85	0.44
1:E:1222:TYR:O	1:E:1223:PHE:C	2.60	0.44
1:E:1265:GLN:O	1:E:1266:GLU:C	2.60	0.44
1:F:1580:GLY:CA	1:F:1643:GLN:NE2	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1717:TYR:CD1	1:F:1717:TYR:N	2.86	0.44
1:G:1992:PHE:CD1	1:G:1992:PHE:C	2.96	0.44
1:B:360:THR:HG23	1:B:360:THR:O	2.18	0.43
1:C:774:PHE:HB2	1:C:782:PHE:CE1	2.53	0.43
1:G:1945:LEU:O	1:G:1946:ASP:C	2.60	0.43
1:A:152:TYR:CE1	1:A:156:ASN:ND2	2.86	0.43
1:C:776:PRO:HD2	1:C:780:GLU:O	2.18	0.43
1:C:807:LEU:HD12	1:C:807:LEU:O	2.17	0.43
1:D:1097:TYR:O	1:D:1100:ILE:HG23	2.17	0.43
1:B:385:HIS:O	1:B:386:LEU:CB	2.65	0.43
1:G:1881:VAL:H	1:G:1943:GLN:NE2	2.15	0.43
1:H:2266:LYS:HB3	1:H:2267:TYR:CE1	2.54	0.43
1:A:94:GLU:OE1	1:B:385:HIS:HB3	2.18	0.43
1:A:129:LEU:C	1:A:129:LEU:CD1	2.91	0.43
1:C:752:TYR:CD1	1:C:756:ASN:ND2	2.86	0.43
1:E:1285:HIS:O	1:E:1286:LEU:CB	2.65	0.43
1:F:1672:ILE:HB	1:F:1686:PHE:CZ	2.53	0.43
1:G:1823:PHE:CE2	1:H:2195:ARG:NE	2.86	0.43
1:H:2258:GLN:CD	1:H:2258:GLN:N	2.76	0.43
1:H:2274:PHE:HB2	1:H:2282:PHE:CE1	2.54	0.43
1:A:177:LYS:HD3	1:A:177:LYS:C	2.44	0.43
1:B:502:LYS:C	1:B:504:ASN:N	2.76	0.43
1:C:656:ASP:O	1:C:657:LYS:HD3	2.19	0.43
1:C:733:ILE:HD13	1:C:749:VAL:HG22	1.99	0.43
1:C:743:GLN:CD	1:C:801:TYR:CD1	2.96	0.43
1:E:1262:LEU:HD23	1:E:1301:GLY:HA2	2.01	0.43
1:E:1341:THR:O	1:E:1342:ALA:C	2.59	0.43
1:E:1361:THR:O	1:E:1363:GLY:N	2.51	0.43
1:F:1516:LYS:HG2	1:F:1690:PRO:O	2.19	0.43
1:F:1615:LYS:HG2	1:F:1709:ASN:ND2	2.34	0.43
1:G:1805:ASP:H	1:G:1808:GLN:CD	2.25	0.43
1:G:1815:VAL:HA	1:G:1990:PRO:HA	2.01	0.43
1:G:1850:VAL:O	1:G:1850:VAL:HG23	2.18	0.43
1:A:146:ASP:OD2	1:A:150:ARG:NE	2.51	0.43
1:C:783:TRP:C	1:C:784:PHE:CD2	2.97	0.43
1:F:1689:GLU:O	1:F:1690:PRO:C	2.62	0.43
1:A:100:TYR:HE2	1:A:199:MET:HG2	1.82	0.43
1:E:1390:PRO:HD2	1:H:2143:SER:CB	2.49	0.43
1:F:1698:LEU:C	1:F:1700:ILE:N	2.74	0.43
1:G:1913:ILE:HD12	1:G:1913:ILE:N	2.34	0.43
1:G:2015:GLU:HB3	1:G:2017:TYR:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2181:VAL:H	1:H:2243:GLN:NE2	2.10	0.43
1:A:94:GLU:O	1:A:95:ARG:HB2	2.19	0.43
1:A:197:TYR:C	1:A:199:MET:N	2.76	0.43
1:B:315:VAL:HA	1:B:490:PRO:HA	2.00	0.43
1:B:421:VAL:HG12	1:B:422:SER:N	2.34	0.43
1:B:446:ASP:OD2	1:B:450:ARG:HG3	2.18	0.43
1:C:641:LEU:HG	1:C:642:LEU:HG	1.99	0.43
1:D:940:GLN:O	1:D:940:GLN:HG3	2.17	0.43
1:D:955:TYR:C	1:D:995:ARG:HH12	2.27	0.43
1:D:977:ASP:OD1	1:D:1006:HIS:CD2	2.71	0.43
1:D:1089:GLU:O	1:D:1090:PRO:C	2.62	0.43
1:E:1232:HIS:CE1	1:E:1250:VAL:HB	2.53	0.43
1:E:1343:GLN:HG3	1:E:1401:TYR:CD1	2.53	0.43
1:F:1570:LEU:O	1:F:1574:LYS:HD3	2.18	0.43
1:B:520:THR:O	1:B:521:LYS:OXT	2.37	0.43
1:D:981:VAL:N	1:D:1043:GLN:NE2	2.59	0.43
1:E:1417:TYR:O	1:E:1418:LEU:HD23	2.18	0.43
1:A:82:GLU:OE1	1:A:82:GLU:N	2.49	0.43
1:B:305:ASP:C	1:B:307:SER:H	2.26	0.43
1:C:645:ASP:OD1	1:C:645:ASP:C	2.61	0.43
1:D:1093:THR:O	1:D:1094:GLN:C	2.62	0.43
1:E:1223:PHE:HE2	1:F:1595:ARG:NH2	2.13	0.43
1:E:1243:SER:HB2	1:H:2289:GLU:HB3	2.01	0.43
1:E:1270:LEU:O	1:E:1274:LYS:HD3	2.19	0.43
1:E:1279:TYR:CD2	1:E:1344:GLU:HA	2.54	0.43
1:E:1311:LEU:HG	1:E:1338:LYS:HG2	2.01	0.43
1:E:1396:LYS:HD3	1:E:1397:TYR:CA	2.48	0.43
1:F:1692:PHE:CD1	1:F:1692:PHE:C	2.96	0.43
1:G:1890:CYS:C	1:G:1892:ASN:N	2.74	0.43
1:H:2104:PRO:HD3	1:H:2283:TRP:CE2	2.54	0.43
1:A:70:LEU:O	1:A:74:LYS:HD3	2.19	0.42
1:A:71:PHE:CD1	1:A:71:PHE:N	2.87	0.42
1:C:632:HIS:CE1	1:C:650:VAL:HB	2.55	0.42
1:C:683:TYR:CE1	1:C:698:CYS:CB	3.01	0.42
1:D:971:PHE:CD1	1:D:971:PHE:N	2.86	0.42
1:D:995:ARG:HB3	1:D:995:ARG:NH1	2.34	0.42
1:H:2179:TYR:CD2	1:H:2244:GLU:CG	3.01	0.42
1:H:2289:GLU:O	1:H:2290:PRO:C	2.62	0.42
1:A:113:ILE:HA	1:A:114:PRO:HD3	1.90	0.42
1:C:615:VAL:HA	1:C:790:PRO:HA	2.01	0.42
1:C:615:VAL:HG13	1:C:792:PHE:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:745:LEU:O	1:C:747:TYR:N	2.52	0.42
1:D:1027:GLN:O	1:D:1027:GLN:HG2	2.19	0.42
1:D:1059:LEU:HG	1:D:1060:TYR:CE2	2.54	0.42
1:E:1377:LYS:HD3	1:E:1377:LYS:C	2.44	0.42
1:F:1565:GLN:O	1:F:1566:GLU:C	2.62	0.42
1:F:1570:LEU:C	1:F:1570:LEU:CD2	2.92	0.42
1:G:1974:PHE:CD1	1:G:1974:PHE:N	2.87	0.42
1:H:2125:TYR:O	1:H:2247:TYR:HE1	2.01	0.42
1:H:2170:LEU:O	1:H:2174:LYS:HD3	2.19	0.42
1:B:332:HIS:CE1	1:B:350:VAL:HB	2.53	0.42
1:B:377:ASP:OD2	1:B:406:HIS:HA	2.19	0.42
1:E:1229:PRO:HD3	1:E:1347:TYR:OH	2.19	0.42
1:E:1285:HIS:CD2	1:E:1286:LEU:HG	2.54	0.42
1:E:1406:THR:HG22	1:E:1407:LEU:N	2.35	0.42
1:F:1700:ILE:HG13	1:F:1701:TYR:CD2	2.54	0.42
1:G:1874:LYS:O	1:G:1876:VAL:HG13	2.19	0.42
1:G:1951:LYS:O	1:G:1954:ILE:HB	2.20	0.42
1:H:2168:ALA:O	1:H:2170:LEU:N	2.52	0.42
1:B:321:ILE:O	1:B:322:TYR:C	2.62	0.42
1:B:380:GLY:HA2	1:B:443:GLN:NE2	2.35	0.42
1:C:698:CYS:O	1:C:699:ILE:CG2	2.66	0.42
1:D:1050:ARG:NH2	1:D:1086:PHE:HD2	2.17	0.42
1:G:1856:ASP:O	1:G:1857:LYS:HD3	2.18	0.42
1:A:108:GLY:O	1:A:109:ASN:HB2	2.18	0.42
1:A:159:LEU:HG	1:A:160:TYR:CE2	2.55	0.42
1:B:508:ASP:OD2	1:B:510:LYS:HB3	2.19	0.42
1:C:680:GLY:HA2	1:C:743:GLN:NE2	2.34	0.42
1:E:1215:VAL:HA	1:E:1390:PRO:HA	2.01	0.42
1:E:1268:ALA:C	1:E:1270:LEU:N	2.76	0.42
1:E:1284:TYR:O	1:E:1285:HIS:C	2.62	0.42
1:G:1952:TYR:C	1:G:1954:ILE:N	2.77	0.42
1:A:175:ILE:HA	1:A:176:PRO:HD3	1.79	0.42
1:B:411:LEU:HB3	1:B:412:GLU:H	1.76	0.42
1:C:695:ARG:NH2	1:D:923:PHE:CE2	2.87	0.42
1:D:1047:TYR:O	1:D:1049:VAL:N	2.52	0.42
1:E:1288:TYR:CD1	1:E:1288:TYR:N	2.88	0.42
1:F:1515:VAL:O	1:F:1516:LYS:O	2.38	0.42
1:F:1706:THR:HG22	1:F:1707:LEU:N	2.34	0.42
1:H:2137:SER:OG	1:H:2172:LYS:O	2.33	0.42
1:A:85:HIS:O	1:A:86:LEU:CB	2.67	0.42
1:B:516:VAL:C	1:B:517:TYR:CD1	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:914:LEU:O	1:D:915:VAL:C	2.63	0.42
1:D:1043:GLN:CD	1:D:1101:TYR:CD1	2.98	0.42
1:E:1210:HIS:CD2	1:E:1210:HIS:H	2.36	0.42
1:F:1631:PHE:C	1:F:1632:ASP:OD2	2.62	0.42
1:F:1702:LYS:O	1:F:1704:ASN:N	2.52	0.42
1:G:1862:LEU:HD12	1:G:1868:ALA:CA	2.46	0.42
1:G:1940:VAL:HG21	1:G:1945:LEU:HD21	2.01	0.42
1:E:1219:GLN:HG2	1:E:1220:ASN:N	2.35	0.42
1:G:1829:PRO:HG3	1:G:1879:TYR:OH	2.20	0.42
1:H:2223:ILE:O	1:H:2224:ASP:HB2	2.19	0.42
1:H:2252:TYR:C	1:H:2254:ILE:H	2.28	0.42
1:A:174:PHE:HB2	1:A:182:PHE:CE1	2.55	0.42
1:B:329:PRO:HD3	1:B:447:TYR:CZ	2.55	0.42
1:B:410:HIS:NE2	1:B:436:ASN:HB3	2.35	0.42
1:B:443:GLN:OE1	1:B:501:TYR:HB3	2.19	0.42
1:B:477:LYS:HD3	1:B:477:LYS:C	2.45	0.42
1:D:974:LYS:O	1:D:976:VAL:HG13	2.20	0.42
1:E:1271:PHE:O	1:E:1272:LYS:C	2.61	0.42
1:H:2131:THR:O	1:H:2132:HIS:CG	2.72	0.42
1:H:2246:ASP:OD2	1:H:2250:ARG:NE	2.53	0.42
1:A:152:TYR:O	1:A:153:THR:C	2.62	0.42
1:A:158:GLN:N	1:A:158:GLN:CD	2.78	0.42
1:B:310:HIS:ND1	1:B:487:PHE:O	2.53	0.42
1:B:329:PRO:HD3	1:B:447:TYR:CE2	2.55	0.42
1:F:1637:LYS:HB2	1:F:1640:VAL:HG12	2.02	0.42
1:F:1715:GLU:HB3	1:F:1717:TYR:CE1	2.55	0.42
1:H:2130:VAL:O	1:H:2179:TYR:HA	2.20	0.42
1:H:2320:THR:O	1:H:2321:LYS:C	2.61	0.42
1:A:31:THR:O	1:A:32:HIS:CG	2.73	0.41
1:A:70:LEU:C	1:A:70:LEU:CD2	2.93	0.41
1:A:170:GLY:HA2	1:A:217:TYR:O	2.20	0.41
1:A:207:LEU:HD12	1:A:207:LEU:O	2.19	0.41
1:B:359:LYS:HG2	1:B:360:THR:N	2.35	0.41
1:B:508:ASP:OD2	1:B:511:THR:HG23	2.20	0.41
1:C:662:LEU:HD12	1:C:668:ALA:HA	2.02	0.41
1:C:751:LYS:CE	1:C:755:ASP:OD2	2.63	0.41
1:D:959:LYS:HG2	1:D:960:THR:N	2.35	0.41
1:D:985:HIS:O	1:D:986:LEU:HB2	2.19	0.41
1:E:1266:GLU:O	1:E:1267:MET:C	2.63	0.41
1:E:1379:LYS:CG	1:E:1380:GLU:H	2.31	0.41
1:F:1720:THR:O	1:F:1721:LYS:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1929:LEU:C	1:G:1929:LEU:CD1	2.93	0.41
1:C:729:LEU:C	1:C:729:LEU:CD1	2.93	0.41
1:C:747:TYR:O	1:C:750:ARG:N	2.53	0.41
1:D:981:VAL:N	1:D:1043:GLN:HE21	2.16	0.41
1:F:1604:THR:CG2	1:F:1641:THR:HG22	2.49	0.41
1:G:1947:TYR:O	1:G:1948:LYS:C	2.63	0.41
1:G:1972:ILE:HG22	1:G:1984:PHE:HB2	2.01	0.41
1:A:79:TYR:CD2	1:A:144:GLU:HG3	2.54	0.41
1:A:192:PHE:CD1	1:A:193:THR:N	2.88	0.41
1:D:1013:ILE:HA	1:D:1014:PRO:HD3	1.87	0.41
1:E:1210:HIS:ND1	1:E:1387:PHE:O	2.54	0.41
1:E:1268:ALA:C	1:E:1270:LEU:H	2.28	0.41
1:G:1885:HIS:C	1:G:1886:LEU:HG	2.45	0.41
1:G:1943:GLN:HG3	1:G:2001:TYR:CD1	2.55	0.41
1:G:1959:LEU:HG	1:G:1960:TYR:CE2	2.55	0.41
1:H:2116:LYS:O	1:H:2117:ASN:C	2.62	0.41
1:H:2153:PRO:HG2	1:H:2154:ASN:H	1.84	0.41
1:H:2212:GLU:C	1:H:2213:ILE:HD12	2.45	0.41
1:H:2250:ARG:O	1:H:2252:TYR:N	2.53	0.41
1:C:670:LEU:HD23	1:C:670:LEU:O	2.20	0.41
1:C:793:THR:O	1:C:794:GLN:C	2.60	0.41
1:D:1087:PHE:CD1	1:D:1087:PHE:N	2.88	0.41
1:E:1223:PHE:HD1	1:E:1223:PHE:H	1.66	0.41
1:F:1716:VAL:C	1:F:1717:TYR:CD1	2.98	0.41
1:G:1816:LYS:HG2	1:G:1990:PRO:O	2.20	0.41
1:H:2317:TYR:CD1	1:H:2317:TYR:N	2.89	0.41
1:A:18:LEU:O	1:A:19:GLN:C	2.62	0.41
1:B:302:GLN:H	1:B:302:GLN:HE21	1.66	0.41
1:C:739:MET:HB3	1:C:806:THR:CG2	2.50	0.41
1:F:1559:LYS:HE2	1:F:1598:CYS:SG	2.60	0.41
1:G:1821:ILE:HG22	1:G:1960:TYR:CE1	2.55	0.41
1:G:1885:HIS:CD2	1:G:1886:LEU:HG	2.55	0.41
1:G:1966:LYS:HB3	1:G:1967:TYR:CE1	2.55	0.41
1:H:2116:LYS:HE2	1:H:2291:GLU:HA	2.02	0.41
1:B:474:PHE:HB2	1:B:482:PHE:CE1	2.56	0.41
1:B:475:ILE:O	1:B:475:ILE:HG22	2.20	0.41
1:C:782:PHE:CZ	1:C:805:GLU:HG2	2.55	0.41
1:D:1068:GLU:HB2	1:D:1121:LYS:OXT	2.21	0.41
1:G:1825:TYR:CZ	1:G:1950:ARG:NH1	2.88	0.41
1:G:1831:THR:O	1:G:1832:HIS:CG	2.73	0.41
1:G:1894:GLU:O	1:G:1895:ARG:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2002:LYS:C	1:G:2004:ASN:H	2.27	0.41
1:H:2194:GLU:O	1:H:2195:ARG:CB	2.68	0.41
1:H:2302:LYS:C	1:H:2304:ASN:N	2.78	0.41
1:A:202:LYS:C	1:A:204:ASN:N	2.78	0.41
1:B:500:ILE:HG13	1:B:501:TYR:CE2	2.55	0.41
1:C:605:ASP:C	1:C:607:SER:H	2.29	0.41
1:C:761:THR:O	1:C:763:GLY:N	2.52	0.41
1:C:767:TYR:CD2	1:C:818:LEU:HB3	2.56	0.41
1:D:1057:LYS:HD3	1:D:1057:LYS:HA	1.92	0.41
1:E:1347:TYR:C	1:E:1349:VAL:N	2.79	0.41
1:F:1629:LEU:C	1:F:1629:LEU:CD1	2.94	0.41
1:A:59:LYS:HG2	1:A:60:THR:N	2.35	0.41
1:A:68:ALA:O	1:A:69:THR:C	2.63	0.41
1:A:90:CYS:HA	1:C:691:GLU:OE2	2.21	0.41
1:B:319:GLN:O	1:B:320:ASN:C	2.62	0.41
1:B:449:VAL:O	1:B:450:ARG:C	2.62	0.41
1:C:621:ILE:HA	1:C:624:LEU:HD12	2.03	0.41
1:E:1202:GLN:N	1:E:1202:GLN:HE21	2.18	0.41
1:E:1221:ILE:O	1:E:1222:TYR:C	2.63	0.41
1:E:1329:LEU:C	1:E:1329:LEU:CD1	2.94	0.41
1:F:1566:GLU:O	1:F:1567:MET:C	2.63	0.41
1:F:1580:GLY:HA2	1:F:1643:GLN:NE2	2.35	0.41
1:F:1637:LYS:H	1:F:1637:LYS:HG3	1.70	0.41
1:F:1698:LEU:C	1:F:1700:ILE:H	2.29	0.41
1:G:1804:PRO:HD3	1:G:1983:TRP:CE2	2.56	0.41
1:G:1940:VAL:O	1:G:2006:THR:HA	2.20	0.41
1:G:2009:ASN:CG	1:G:2010:LYS:N	2.79	0.41
1:H:2272:ILE:O	1:H:2272:ILE:HG23	2.21	0.41
1:H:2277:LYS:HD3	1:H:2277:LYS:C	2.43	0.41
1:A:141:THR:O	1:A:142:ALA:C	2.63	0.41
1:B:423:ILE:O	1:B:424:ASP:HB2	2.21	0.41
1:C:679:TYR:CE2	1:C:744:GLU:HA	2.55	0.41
1:D:917:ASN:HB3	1:D:920:ASN:ND2	2.36	0.41
1:D:1070:GLY:O	1:D:1086:PHE:HB2	2.21	0.41
1:F:1558:LEU:HA	1:F:1597:ALA:O	2.21	0.41
1:F:1627:GLN:O	1:F:1627:GLN:HG2	2.21	0.41
1:F:1709:ASN:ND2	1:F:1710:LYS:N	2.68	0.41
1:G:1943:GLN:CD	1:G:2001:TYR:CD1	2.99	0.41
1:B:381:VAL:H	1:B:443:GLN:NE2	2.18	0.40
1:B:383:TYR:HB2	1:B:494:GLN:HE21	1.86	0.40
1:B:413:ILE:HA	1:B:414:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:617:ASN:HB3	1:C:619:GLN:OE1	2.21	0.40
1:C:631:THR:O	1:C:632:HIS:CG	2.73	0.40
1:C:679:TYR:CD2	1:C:744:GLU:HG3	2.57	0.40
1:C:752:TYR:CE1	1:C:756:ASN:ND2	2.89	0.40
1:E:1265:GLN:O	1:E:1268:ALA:HB3	2.21	0.40
1:F:1621:VAL:O	1:F:1627:GLN:HG3	2.20	0.40
1:G:1823:PHE:N	1:G:1823:PHE:CD1	2.89	0.40
1:H:2308:ASP:OD2	1:H:2311:THR:HG23	2.21	0.40
1:A:23:PHE:CD1	1:A:23:PHE:N	2.88	0.40
1:E:1234:ASN:OD1	1:E:1275:ASN:HB3	2.21	0.40
1:F:1534:ASN:OD1	1:F:1575:ASN:HB3	2.21	0.40
1:G:1882:GLU:CA	1:G:1899:ILE:HG22	2.45	0.40
1:G:1952:TYR:CE1	1:G:1956:ASN:ND2	2.90	0.40
1:A:183:TRP:C	1:A:184:PHE:CD2	3.00	0.40
1:B:316:LYS:HE2	1:B:492:PHE:N	2.33	0.40
1:D:966:GLU:H	1:D:966:GLU:CD	2.26	0.40
1:F:1708:ASP:OD2	1:F:1711:THR:HG23	2.21	0.40
1:G:1900:TYR:N	1:G:1900:TYR:CD1	2.90	0.40
1:H:2115:VAL:HA	1:H:2290:PRO:HA	2.03	0.40
1:H:2302:LYS:C	1:H:2304:ASN:H	2.29	0.40
1:A:197:TYR:C	1:A:199:MET:H	2.30	0.40
1:C:616:LYS:O	1:C:618:LEU:N	2.55	0.40
1:C:792:PHE:CD1	1:C:792:PHE:C	2.99	0.40
1:C:816:VAL:C	1:C:817:TYR:CD1	3.00	0.40
1:E:1219:GLN:C	1:E:1221:ILE:N	2.79	0.40
1:F:1687:PHE:CD1	1:F:1687:PHE:N	2.90	0.40
1:G:1923:ILE:O	1:G:1924:ASP:HB2	2.20	0.40
1:G:1977:LYS:HD3	1:G:1977:LYS:C	2.46	0.40
1:H:2146:LEU:HD23	1:H:2146:LEU:HA	1.84	0.40
1:H:2247:TYR:O	1:H:2248:LYS:C	2.65	0.40
1:A:95:ARG:NH1	1:A:95:ARG:CB	2.84	0.40
1:A:109:ASN:O	1:A:137:LYS:HA	2.22	0.40
1:A:126:ILE:H	1:A:126:ILE:HG12	1.74	0.40
1:A:174:PHE:CD1	1:A:174:PHE:N	2.90	0.40
1:F:1682:PHE:C	1:F:1682:PHE:CD1	3.00	0.40
1:H:2129:PRO:HD3	1:H:2247:TYR:OH	2.21	0.40
1:H:2171:PHE:CD1	1:H:2171:PHE:N	2.90	0.40
1:H:2228:SER:O	1:H:2229:LEU:HB3	2.22	0.40
1:H:2283:TRP:O	1:H:2284:PHE:HD2	2.05	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	219/221 (99%)	164 (75%)	40 (18%)	15 (7%)	1	14
1	B	219/221 (99%)	168 (77%)	35 (16%)	16 (7%)	1	13
1	C	219/221 (99%)	172 (78%)	34 (16%)	13 (6%)	1	15
1	D	219/221 (99%)	171 (78%)	37 (17%)	11 (5%)	1	18
1	E	219/221 (99%)	163 (74%)	46 (21%)	10 (5%)	2	19
1	F	219/221 (99%)	160 (73%)	50 (23%)	9 (4%)	2	20
1	G	219/221 (99%)	178 (81%)	31 (14%)	10 (5%)	2	19
1	H	219/221 (99%)	173 (79%)	34 (16%)	12 (6%)	1	17
All	All	1752/1768 (99%)	1349 (77%)	307 (18%)	96 (6%)	1	17

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	B	316	LYS
1	B	334	ASN
1	D	916	LYS
1	E	1216	LYS
1	F	1516	LYS
1	G	1816	LYS
1	H	2116	LYS
1	A	16	LYS
1	A	17	ASN
1	A	86	LEU
1	B	322	TYR
1	B	386	LEU
1	B	443	GLN
1	C	616	LYS
1	C	634	ASN
1	C	643	SER

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Mol	Chain	Res	Type
1	C	686	LEU
1	C	744	GLU
1	D	934	ASN
1	D	943	SER
1	D	1047	TYR
1	D	1098	LEU
1	E	1234	ASN
1	E	1286	LEU
1	F	1534	ASN
1	F	1543	SER
1	F	1586	LEU
1	F	1609	ASN
1	F	1644	GLU
1	F	1710	LYS
1	G	1843	SER
1	G	1886	LEU
1	H	2117	ASN
1	H	2143	SER
1	H	2186	LEU
1	H	2298	LEU
1	A	34	ASN
1	A	144	GLU
1	A	145	LEU
1	A	146	ASP
1	B	368	ALA
1	B	405	ASN
1	B	409	ASN
1	B	444	GLU
1	B	453	THR
1	C	695	ARG
1	C	743	GLN
1	C	745	LEU
1	D	995	ARG
1	D	1009	ASN
1	D	1048	LYS
1	E	1217	ASN
1	E	1309	ASN
1	E	1410	LYS
1	F	1541	LEU
1	F	1652	TYR
1	G	1895	ARG
1	G	1952	TYR

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Mol	Chain	Res	Type
1	H	2106	PRO
1	H	2251	LYS
1	H	2253	THR
1	A	143	GLN
1	A	152	TYR
1	A	159	LEU
1	B	306	PRO
1	B	452	TYR
1	B	498	LEU
1	C	705	ASN
1	C	752	TYR
1	C	759	LEU
1	D	1043	GLN
1	D	1044	GLU
1	E	1206	PRO
1	E	1222	TYR
1	E	1297	ALA
1	E	1352	TYR
1	G	1909	ASN
1	G	1953	THR
1	H	2134	ASN
1	H	2205	ASN
1	H	2209	ASN
1	A	68	ALA
1	A	198	LEU
1	A	210	LYS
1	B	445	LEU
1	C	637	SER
1	C	746	ASP
1	H	2169	THR
1	A	15	VAL
1	B	323	PHE
1	B	451	LYS
1	D	986	LEU
1	G	1817	ASN
1	G	1834	ASN
1	G	1943	GLN

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	208/208 (100%)	200 (96%)	8 (4%)	29	52
1	B	208/208 (100%)	203 (98%)	5 (2%)	43	63
1	C	208/208 (100%)	205 (99%)	3 (1%)	59	71
1	D	208/208 (100%)	202 (97%)	6 (3%)	37	58
1	E	208/208 (100%)	204 (98%)	4 (2%)	50	66
1	F	208/208 (100%)	203 (98%)	5 (2%)	43	63
1	G	208/208 (100%)	201 (97%)	7 (3%)	32	55
1	H	208/208 (100%)	200 (96%)	8 (4%)	29	52
All	All	1664/1664 (100%)	1618 (97%)	46 (3%)	38	59

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	19	GLN
1	A	36	LYS
1	A	82	GLU
1	A	88	TYR
1	A	107	GLU
1	A	129	LEU
1	A	167	TYR
1	B	302	GLN
1	B	319	GLN
1	B	336	LYS
1	B	382	GLU
1	B	490	PRO
1	C	602	GLN
1	C	619	GLN
1	C	682	GLU
1	D	902	GLN
1	D	919	GLN
1	D	982	GLU
1	D	988	TYR
1	D	1007	GLU
1	D	1090	PRO
1	E	1202	GLN

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Mol	Chain	Res	Type
1	E	1219	GLN
1	E	1282	GLU
1	E	1307	GLU
1	F	1502	GLN
1	F	1519	GLN
1	F	1582	GLU
1	F	1588	TYR
1	F	1607	GLU
1	G	1802	GLN
1	G	1819	GLN
1	G	1882	GLU
1	G	1888	TYR
1	G	1929	LEU
1	G	1932	ASP
1	G	1967	TYR
1	H	2102	GLN
1	H	2119	GLN
1	H	2182	GLU
1	H	2188	TYR
1	H	2207	GLU
1	H	2229	LEU
1	H	2267	TYR
1	H	2290	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	2	GLN
1	A	8	GLN
1	A	19	GLN
1	A	40	GLN
1	A	85	HIS
1	A	92	ASN
1	A	106	HIS
1	A	143	GLN
1	A	156	ASN
1	A	194	GLN
1	B	301	GLN
1	B	302	GLN
1	B	308	GLN
1	B	319	GLN

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Mol	Chain	Res	Type
1	B	344	HIS
1	B	365	GLN
1	B	375	ASN
1	B	385	HIS
1	B	406	HIS
1	B	427	GLN
1	B	436	ASN
1	B	443	GLN
1	B	456	ASN
1	B	494	GLN
1	B	509	ASN
1	C	602	GLN
1	C	608	GLN
1	C	619	GLN
1	C	640	GLN
1	C	649	ASN
1	C	685	HIS
1	C	706	HIS
1	C	743	GLN
1	C	756	ASN
1	C	794	GLN
1	C	809	ASN
1	D	902	GLN
1	D	908	GLN
1	D	919	GLN
1	D	920	ASN
1	D	940	GLN
1	D	985	HIS
1	D	1006	HIS
1	D	1027	GLN
1	D	1043	GLN
1	D	1094	GLN
1	E	1202	GLN
1	E	1208	GLN
1	E	1219	GLN
1	E	1220	ASN
1	E	1240	GLN
1	E	1285	HIS
1	E	1327	GLN
1	E	1343	GLN
1	E	1394	GLN
1	F	1502	GLN

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Mol	Chain	Res	Type
1	F	1508	GLN
1	F	1519	GLN
1	F	1540	GLN
1	F	1575	ASN
1	F	1585	HIS
1	F	1592	ASN
1	F	1627	GLN
1	F	1643	GLN
1	F	1656	ASN
1	F	1658	GLN
1	F	1662	ASN
1	F	1694	GLN
1	F	1709	ASN
1	G	1801	GLN
1	G	1802	GLN
1	G	1808	GLN
1	G	1819	GLN
1	G	1885	HIS
1	G	1906	HIS
1	G	1927	GLN
1	G	1943	GLN
1	G	1956	ASN
1	G	1958	GLN
1	G	1994	GLN
1	G	2009	ASN
1	H	2102	GLN
1	H	2108	GLN
1	H	2119	GLN
1	H	2120	ASN
1	H	2140	GLN
1	H	2149	ASN
1	H	2185	HIS
1	H	2206	HIS
1	H	2236	ASN
1	H	2243	GLN
1	H	2256	ASN
1	H	2258	GLN
1	H	2294	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.