



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:29 PM UTC

PDB ID : 3TYH / pdb_00003tyh
Title : Crystal structure of oxo-copper clusters binding to ferric binding protein from *Neisseria gonorrhoeae*
Authors : Chen, W.J.; Wang, H.F.; Zhou, C.J.; Ye, D.R.; Huang, J.; Tan, X.S.; Zhong, W.Q.
Deposited on : 2011-09-26
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

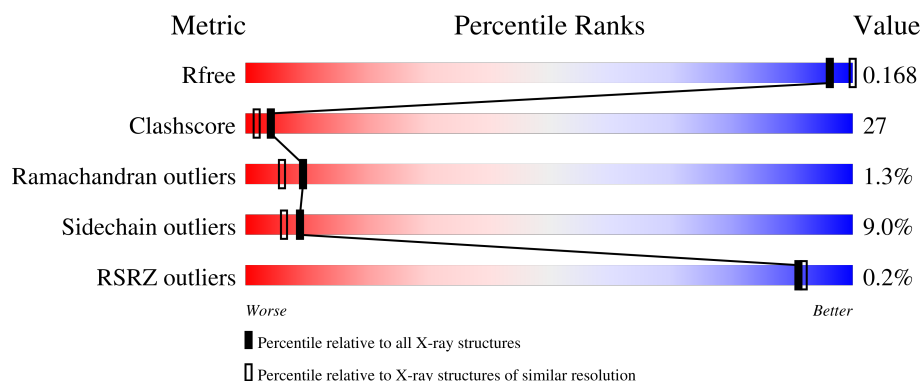
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	309	
1	B	309	
1	C	309	
1	D	309	
1	E	309	

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Mol	Chain	Length	Quality of chain
1	F	309	59%36%5%
1	G	309	57%37%6%
1	H	309	% 44%47%8%
1	I	309	46%46%8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22889 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 FbpA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	B	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	C	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	D	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	E	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	F	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	G	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	H	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	I	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		
2	C	2	Total	Cu	0	0
			2	2		
2	D	2	Total	Cu	0	0
			2	2		
2	E	2	Total	Cu	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	2	Total 2	Cu 2	0	0
2	G	2	Total 2	Cu 2	0	0
2	H	2	Total 2	Cu 2	0	0
2	I	2	Total 2	Cu 2	0	0

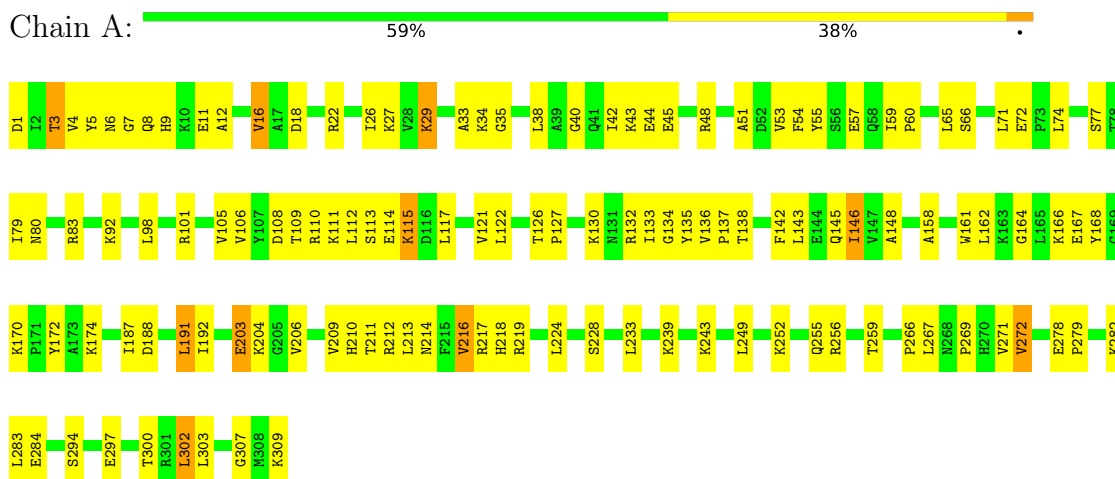
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	217	Total 217	O 217	0	0
3	B	166	Total 166	O 166	0	0
3	C	188	Total 188	O 188	0	0
3	D	177	Total 177	O 177	0	0
3	E	178	Total 178	O 178	0	0
3	F	181	Total 181	O 181	0	0
3	G	123	Total 123	O 123	0	0
3	H	120	Total 120	O 120	0	0
3	I	119	Total 119	O 119	0	0

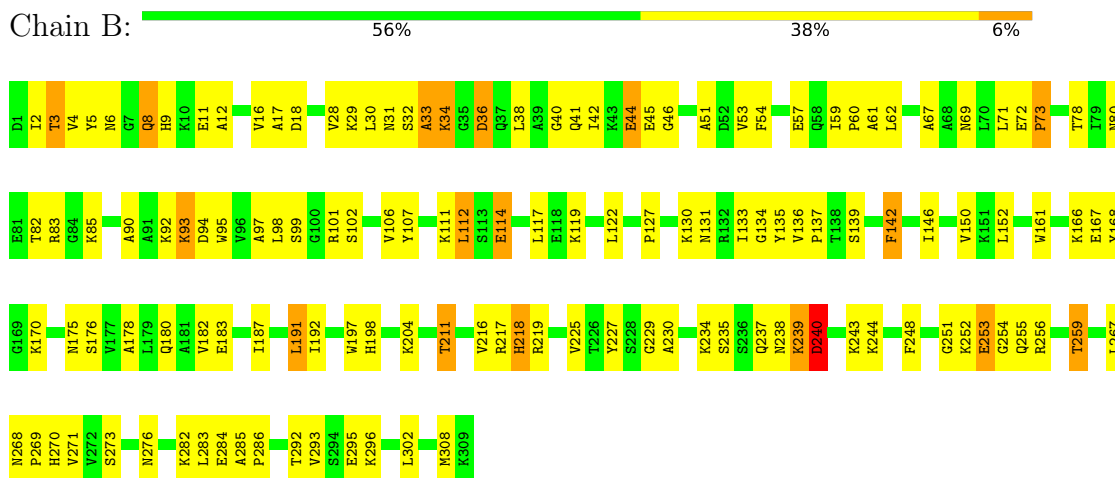
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: FbpA protein

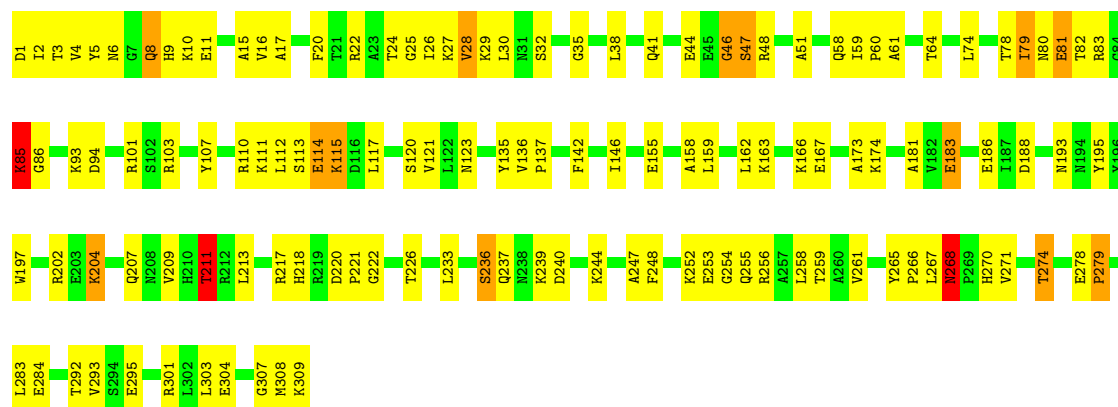


• Molecule 1: FbpA protein



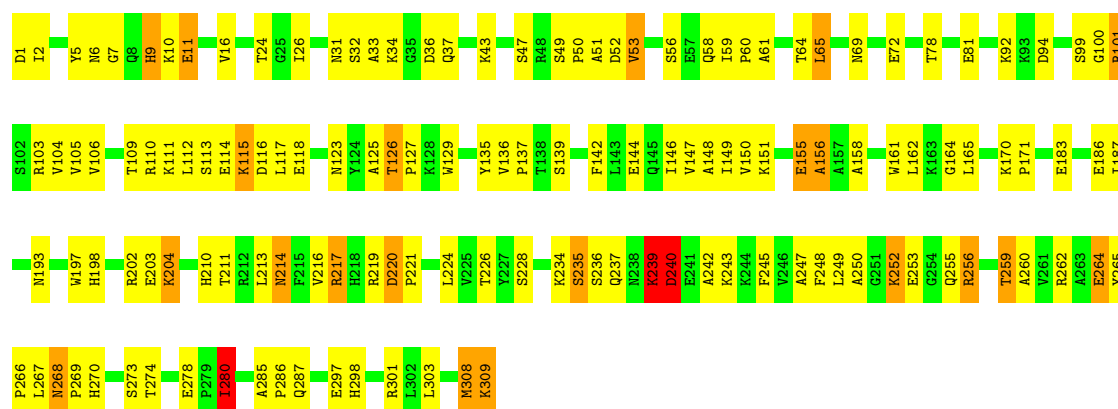
• Molecule 1: FbpA protein





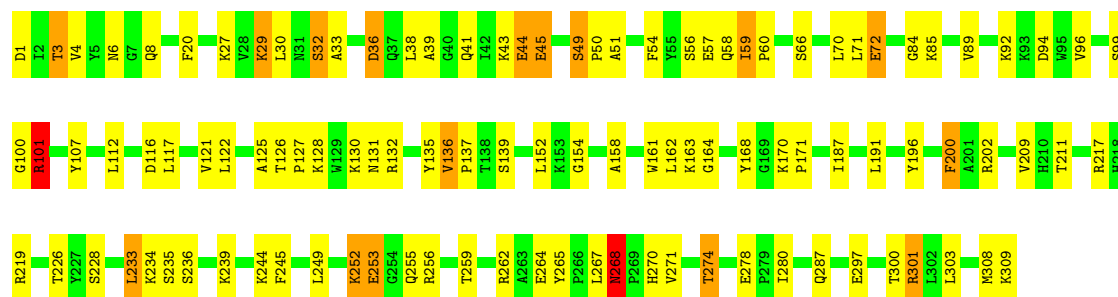
• Molecule 1: FbpA protein

Chain D: 54% 38% 7% •



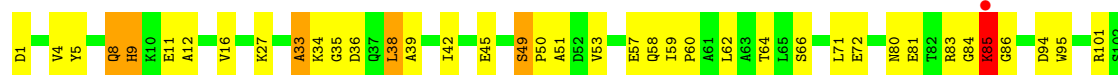
• Molecule 1: FbpA protein

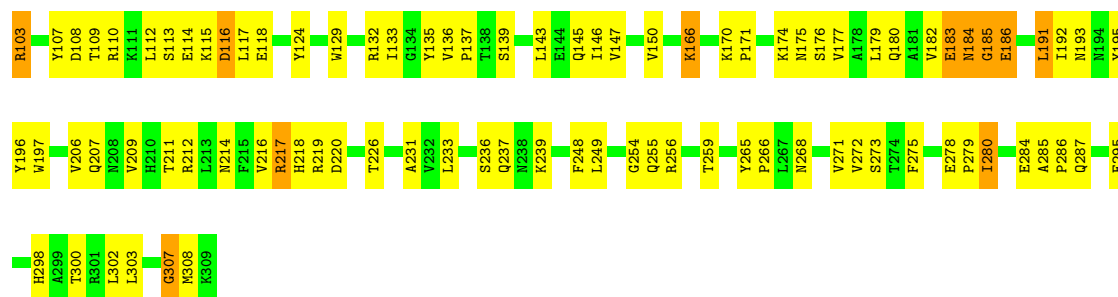
Chain E: 65% 29% 5% •



• Molecule 1: FbpA protein

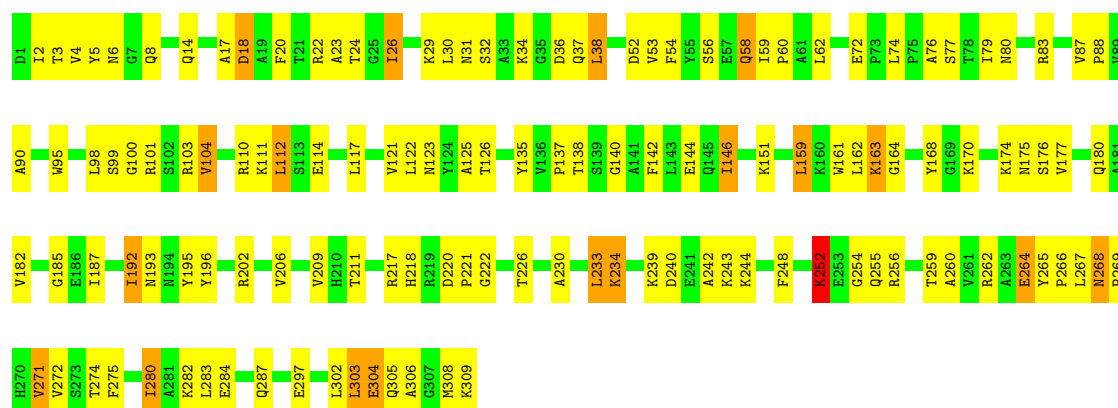
Chain F: 59% 36% 5%





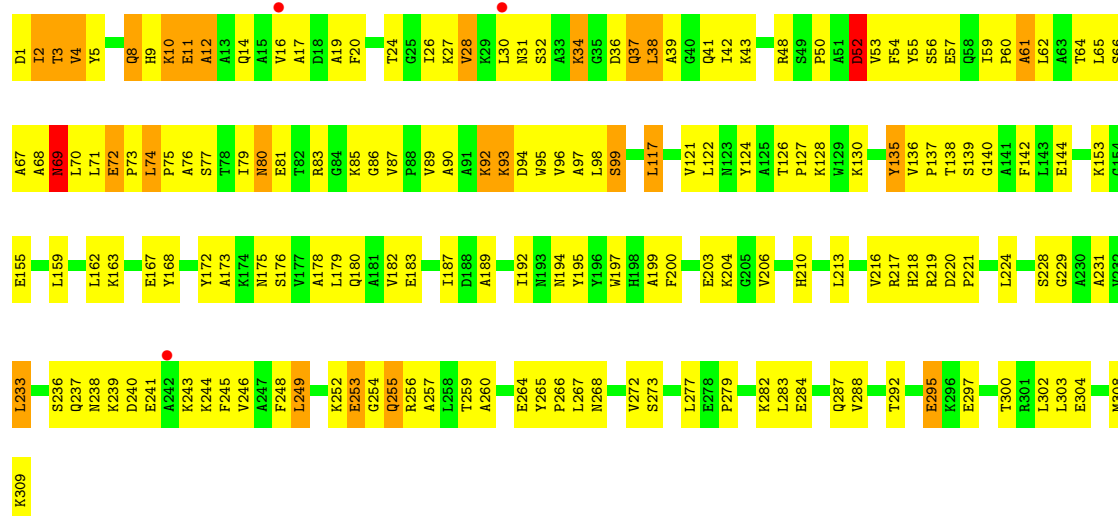
• Molecule 1: FbpA protein

Chain G: 57% 37% 6%



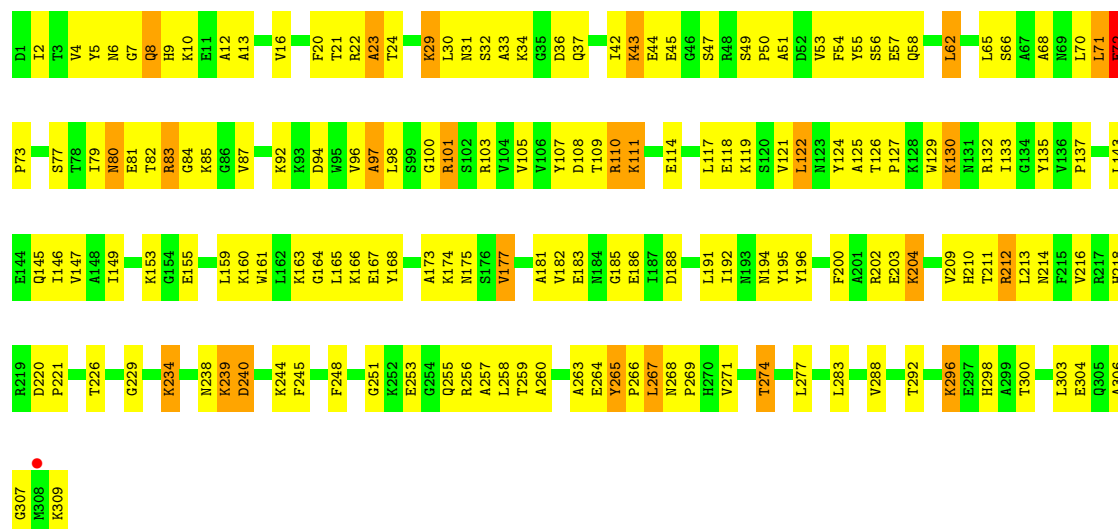
• Molecule 1: FbpA protein

Chain H: 44% 47% 8%



• Molecule 1: FbpA protein

Chain I: 46% 46% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	146.51Å 146.51Å 114.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.96 – 2.10 47.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.96-2.10) 99.9 (47.96-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.143 , 0.169 0.146 , 0.168	Depositor DCC
R_{free} test set	8174 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l 0.018 for h,-h-k,-l 0.045 for -k,-h,-l	Xtriage
Reported twinning fraction	0.541 for H, K, L 0.459 for h+k,-k,-l	Depositor
Outliers	0 of 160455 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22889	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.81	0/2423	1.20	1/3280 (0.0%)
1	B	0.78	0/2423	1.25	6/3280 (0.2%)
1	C	0.77	0/2423	1.26	13/3280 (0.4%)
1	D	0.72	0/2423	1.25	10/3280 (0.3%)
1	E	0.76	0/2423	1.23	13/3280 (0.4%)
1	F	0.87	5/2423 (0.2%)	1.30	12/3280 (0.4%)
1	G	0.63	0/2423	1.20	11/3280 (0.3%)
1	H	0.56	0/2423	1.26	14/3280 (0.4%)
1	I	0.58	0/2423	1.22	14/3280 (0.4%)
All	All	0.73	5/21807 (0.0%)	1.24	94/29520 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	85	LYS	C-N	-7.84	1.22	1.33
1	F	84	GLY	C-N	-6.95	1.24	1.33
1	F	83	ARG	C-O	-6.17	1.16	1.23
1	F	85	LYS	C-O	-5.75	1.16	1.24
1	F	86	GLY	C-O	-5.43	1.16	1.23

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	84	GLY	O-C-N	-9.93	111.59	123.61
1	H	74	LEU	CA-C-N	9.71	130.47	119.99
1	H	74	LEU	C-N-CA	9.71	130.47	119.99
1	F	85	LYS	CA-C-N	-9.26	103.27	121.41
1	F	85	LYS	C-N-CA	-9.26	103.27	121.41
1	D	49	SER	CA-C-N	9.17	129.77	119.32
1	D	49	SER	C-N-CA	9.17	129.77	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	268	ASN	CA-C-N	8.50	128.23	119.56
1	G	268	ASN	C-N-CA	8.50	128.23	119.56
1	F	85	LYS	O-C-N	8.33	133.67	122.59
1	H	72	GLU	CA-C-N	8.17	129.26	120.11
1	H	72	GLU	C-N-CA	8.17	129.26	120.11
1	F	84	GLY	CA-C-N	7.96	136.75	121.54
1	F	84	GLY	C-N-CA	7.96	136.75	121.54
1	F	49	SER	CA-C-N	7.89	127.96	119.28
1	F	49	SER	C-N-CA	7.89	127.96	119.28
1	B	18	ASP	N-CA-C	-7.70	102.83	111.07
1	I	265	TYR	CA-C-N	7.16	127.42	119.90
1	I	265	TYR	C-N-CA	7.16	127.42	119.90
1	C	136	VAL	CA-C-N	7.16	127.77	119.47
1	C	136	VAL	C-N-CA	7.16	127.77	119.47
1	D	136	VAL	CA-C-N	7.05	127.35	119.32
1	D	136	VAL	C-N-CA	7.05	127.35	119.32
1	C	4	VAL	N-CA-C	7.04	118.03	107.75
1	E	136	VAL	CA-C-N	6.97	128.56	119.84
1	E	136	VAL	C-N-CA	6.97	128.56	119.84
1	H	52	ASP	N-CA-C	-6.96	105.41	114.04
1	E	72	GLU	CA-C-N	6.88	126.91	119.90
1	E	72	GLU	C-N-CA	6.88	126.91	119.90
1	D	126	THR	CA-C-N	6.66	126.61	119.28
1	D	126	THR	C-N-CA	6.66	126.61	119.28
1	I	87	VAL	CA-C-N	6.63	127.67	119.98
1	I	87	VAL	C-N-CA	6.63	127.67	119.98
1	I	110	ARG	N-CA-C	-6.62	104.92	114.12
1	H	61	ALA	N-CA-C	-6.47	104.32	111.82
1	F	85	LYS	N-CA-C	6.42	124.48	110.80
1	B	142	PHE	N-CA-C	-6.33	104.46	111.36
1	H	67	ALA	N-CA-C	-6.18	105.43	114.39
1	E	268	ASN	CA-C-N	6.14	125.76	119.56
1	E	268	ASN	C-N-CA	6.14	125.76	119.56
1	H	179	LEU	N-CA-C	-6.05	104.69	111.28
1	I	194	ASN	N-CA-C	6.05	117.95	111.36
1	E	154	GLY	N-CA-C	-6.00	105.57	112.29
1	E	236	SER	N-CA-C	5.95	118.88	109.96
1	D	280	ILE	CB-CA-C	-5.94	104.26	112.04
1	E	59	ILE	CB-CA-C	-5.84	108.16	114.35
1	C	217	ARG	CB-CA-C	-5.82	108.21	115.89
1	C	103	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	I	42	ILE	N-CA-C	5.79	116.53	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	146	ILE	CB-CA-C	-5.77	104.43	111.87
1	C	236	SER	N-CA-C	5.73	117.39	111.03
1	B	62	LEU	N-CA-C	-5.72	106.43	113.41
1	I	72	GLU	CA-C-N	5.70	125.70	119.89
1	I	72	GLU	C-N-CA	5.70	125.70	119.89
1	H	28	VAL	N-CA-C	5.63	115.65	107.88
1	I	166	LYS	N-CA-C	-5.62	104.79	111.03
1	B	36	ASP	N-CA-C	-5.54	106.36	113.23
1	E	49	SER	CA-C-N	5.52	125.19	119.56
1	E	49	SER	C-N-CA	5.52	125.19	119.56
1	G	170	LYS	CA-C-N	5.52	125.28	119.76
1	G	170	LYS	C-N-CA	5.52	125.28	119.76
1	I	97	ALA	N-CA-C	-5.51	102.73	110.50
1	E	101	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	I	23	ALA	N-CA-C	-5.46	108.40	114.62
1	E	139	SER	N-CA-C	5.45	118.22	110.10
1	F	307	GLY	N-CA-C	-5.42	105.54	114.76
1	G	269	PRO	N-CA-C	5.42	120.89	113.84
1	B	102	SER	N-CA-C	5.42	118.23	109.40
1	H	31	ASN	N-CA-C	-5.41	101.65	110.20
1	C	110	ARG	N-CA-C	-5.40	106.64	113.18
1	F	217	ARG	CB-CA-C	-5.38	108.78	115.89
1	D	220	ASP	CA-C-N	-5.38	113.49	119.19
1	D	220	ASP	C-N-CA	-5.38	113.49	119.19
1	B	150	VAL	CB-CA-C	-5.36	104.90	112.14
1	A	6	ASN	N-CA-C	5.34	118.13	107.62
1	I	101	ARG	N-CA-C	-5.29	101.08	109.59
1	D	202	ARG	N-CA-C	-5.28	105.43	111.14
1	G	103	ARG	N-CA-C	-5.25	103.09	110.50
1	C	74	LEU	CA-C-N	5.24	125.16	119.76
1	C	74	LEU	C-N-CA	5.24	125.16	119.76
1	H	122	LEU	N-CA-C	-5.22	105.65	112.23
1	G	36	ASP	N-CA-C	-5.19	105.75	111.71
1	G	252	LYS	N-CA-C	5.18	117.34	111.02
1	G	271	VAL	N-CA-C	5.18	115.72	108.89
1	F	207	GLN	N-CA-C	-5.14	106.51	112.89
1	H	4	VAL	N-CA-C	5.14	114.98	107.37
1	C	211	THR	CB-CA-C	5.13	118.09	109.48
1	C	32	SER	N-CA-C	5.12	117.25	108.90
1	C	268	ASN	CA-C-N	5.12	124.78	119.56
1	C	268	ASN	C-N-CA	5.12	124.78	119.56
1	G	123	ASN	N-CA-C	5.11	119.14	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	140	GLY	N-CA-C	-5.06	108.38	114.66
1	G	260	ALA	N-CA-C	-5.03	107.00	113.23
1	H	302	LEU	N-CA-C	-5.02	106.00	111.82

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	2378	0	2424	126	0
1	B	2378	0	2424	120	0
1	C	2378	0	2424	114	0
1	D	2378	0	2424	156	0
1	E	2378	0	2424	88	0
1	F	2378	0	2424	137	0
1	G	2378	0	2425	115	0
1	H	2378	0	2424	178	0
1	I	2378	0	2424	156	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
3	A	217	0	0	17	0
3	B	166	0	0	14	0
3	C	188	0	0	11	0
3	D	177	0	0	19	0
3	E	178	0	0	3	0
3	F	181	0	0	16	0
3	G	123	0	0	8	0
3	H	120	0	0	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	119	0	0	17	0
All	All	22889	0	21817	1183	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 27.

All (1183) 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:252:LYS:HE2	1:B:256:ARG:NH2	1.45	1.30
1:C:202:ARG:HH22	1:C:274:THR:HG23	1.07	1.12
1:A:284:GLU:HB3	3:A:1406:HOH:O	1.49	1.11
1:I:202:ARG:HH22	1:I:274:THR:HG23	1.14	1.11
1:F:192:ILE:HG22	1:F:193:ASN:H	1.13	1.08
1:E:202:ARG:HH22	1:E:274:THR:HG23	0.93	1.06
1:A:279:PRO:HD2	1:A:282:LYS:HE2	1.34	1.05
1:C:121:VAL:HG21	1:C:222:GLY:HA3	1.32	1.04
1:H:80:ASN:HA	1:H:83:ARG:HD3	1.39	1.04
1:A:101:ARG:HH22	1:A:228:SER:HB3	1.22	1.01
1:D:125:ALA:HB1	1:D:164:GLY:HA3	1.42	1.00
1:F:308:MET:O	1:F:308:MET:HG2	1.60	1.00
1:B:4:VAL:HG22	1:B:53:VAL:HB	1.43	0.98
1:H:54:PHE:HB3	1:H:231:ALA:HB3	1.45	0.98
1:E:202:ARG:NH2	1:E:274:THR:HG23	1.79	0.98
1:G:202:ARG:NH2	1:G:274:THR:HG22	1.79	0.97
1:H:1:ASP:OD1	1:H:27:LYS:HB2	1.64	0.97
1:F:265:TYR:HB3	1:F:280:ILE:HG12	1.45	0.97
1:E:170:LYS:HD2	1:E:187:ILE:HD12	1.43	0.97
1:B:197:TRP:NE1	1:B:211:THR:HG22	1.82	0.95
1:F:85:LYS:CE	1:F:219:ARG:HH22	1.80	0.94
1:A:146:ILE:HD13	1:A:162:LEU:HD11	1.49	0.93
1:B:197:TRP:HE1	1:B:211:THR:HG22	1.27	0.93
1:I:304:GLU:HG2	1:I:309:LYS:OXT	1.67	0.93
1:H:303:LEU:HB3	1:H:309:LYS:HG3	1.48	0.93
1:H:32:SER:HA	3:H:1604:HOH:O	1.68	0.92
1:B:252:LYS:HE2	1:B:256:ARG:HH21	1.11	0.92
1:H:80:ASN:CA	1:H:83:ARG:HD3	2.00	0.92
1:F:133:ILE:HB	3:F:1325:HOH:O	1.68	0.92
1:H:99:SER:HA	1:H:267:LEU:HG	1.52	0.92
1:F:192:ILE:HG22	1:F:193:ASN:N	1.81	0.91
1:C:121:VAL:CG2	1:C:222:GLY:HA3	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:ALA:HB1	1:H:28:VAL:HG21	1.52	0.89
1:A:279:PRO:HD2	1:A:282:LYS:CE	2.03	0.89
1:C:303:LEU:HD12	1:C:308:MET:HE3	1.53	0.89
1:A:101:ARG:NH2	1:A:228:SER:HB3	1.88	0.88
1:E:72:GLU:HG2	1:E:234:LYS:HA	1.56	0.88
1:C:202:ARG:HH22	1:C:274:THR:CG2	1.87	0.88
1:I:200:PHE:CE1	1:I:204:LYS:HG3	2.09	0.88
1:D:267:LEU:HA	1:D:280:ILE:HD11	1.56	0.87
1:F:85:LYS:NZ	1:F:219:ARG:HH22	1.70	0.87
1:I:56:SER:HB3	3:I:1137:HOH:O	1.74	0.87
1:H:80:ASN:C	1:H:83:ARG:HD3	2.00	0.86
1:A:111:LYS:O	1:A:112:LEU:HD23	1.75	0.86
1:H:4:VAL:HG22	1:H:53:VAL:HB	1.54	0.86
1:I:159:LEU:HD11	1:I:163:LYS:HE3	1.57	0.86
1:B:252:LYS:CE	1:B:256:ARG:NH2	2.36	0.86
1:C:202:ARG:NH2	1:C:274:THR:HG23	1.90	0.85
1:F:147:VAL:HG22	1:F:295:GLU:HG3	1.58	0.85
1:I:125:ALA:HB1	1:I:164:GLY:HA3	1.56	0.85
1:A:278:GLU:HB3	1:A:282:LYS:HE2	1.58	0.85
1:F:85:LYS:HZ3	1:F:219:ARG:NH2	1.73	0.85
1:A:9:HIS:HD2	1:A:11:GLU:H	1.25	0.85
1:F:110:ARG:HH22	1:F:183:GLU:C	1.83	0.85
1:H:303:LEU:HD13	1:H:309:LYS:HD2	1.59	0.85
1:F:85:LYS:NZ	1:F:219:ARG:NH2	2.25	0.84
1:B:80:ASN:OD1	1:B:83:ARG:HD3	1.77	0.84
1:D:101:ARG:HH12	1:D:264:GLU:CG	1.91	0.84
1:I:127:PRO:HA	1:I:130:LYS:HG3	1.58	0.84
1:F:275:PHE:HD1	3:F:1091:HOH:O	1.60	0.83
1:F:85:LYS:HE2	1:F:219:ARG:HH22	1.41	0.83
1:G:256:ARG:NH2	1:G:272:VAL:H	1.76	0.83
1:E:202:ARG:HH22	1:E:274:THR:CG2	1.87	0.83
1:C:162:LEU:HD22	1:C:308:MET:HE1	1.60	0.83
1:G:202:ARG:HH22	1:G:274:THR:HG22	1.42	0.83
1:H:38:LEU:O	1:H:42:ILE:HD12	1.79	0.83
1:I:259:THR:CG2	1:I:266:PRO:HG3	2.09	0.83
1:C:61:ALA:O	1:C:64:THR:HG22	1.78	0.83
1:F:192:ILE:CG2	1:F:193:ASN:H	1.90	0.82
1:F:129:TRP:HB3	3:F:1325:HOH:O	1.80	0.82
1:E:262:ARG:HG3	1:E:264:GLU:HG3	1.60	0.81
1:A:252:LYS:HE2	1:A:256:ARG:HH12	1.45	0.81
1:D:101:ARG:NH1	1:D:264:GLU:HG2	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:82:THR:HB	1:I:267:LEU:HB3	1.61	0.81
1:B:41:GLN:HA	1:B:44:GLU:OE2	1.80	0.81
1:D:101:ARG:HH12	1:D:264:GLU:HG2	1.46	0.81
1:H:62:LEU:HD13	1:H:95:TRP:HB2	1.63	0.81
1:A:278:GLU:HB3	1:A:282:LYS:CE	2.11	0.80
1:H:259:THR:HG21	1:H:266:PRO:HG3	1.62	0.80
1:D:101:ARG:NH1	1:D:264:GLU:CB	2.45	0.80
1:G:104:VAL:HG12	1:G:192:ILE:HG13	1.63	0.80
1:G:304:GLU:HA	1:G:309:LYS:HB2	1.64	0.80
1:H:182:VAL:HG22	3:H:1274:HOH:O	1.82	0.80
1:H:220:ASP:OD1	1:H:221:PRO:HD2	1.80	0.80
1:A:115:LYS:HB2	1:A:115:LYS:NZ	1.96	0.79
1:F:147:VAL:HG13	1:F:295:GLU:HG2	1.62	0.79
1:F:265:TYR:HB3	1:F:280:ILE:CG1	2.12	0.79
1:E:196:TYR:O	1:E:200:PHE:CD1	2.35	0.79
1:F:129:TRP:HE3	3:F:1325:HOH:O	1.65	0.79
1:G:5:TYR:HE1	1:G:31:ASN:HD22	1.29	0.79
1:B:5:TYR:CE1	1:B:51:ALA:HB2	2.17	0.79
1:I:182:VAL:HG13	1:I:211:THR:HG21	1.64	0.79
1:H:20:PHE:CE1	1:H:24:THR:HG21	2.18	0.79
1:B:252:LYS:CE	1:B:256:ARG:HH21	1.95	0.78
1:D:11:GLU:CD	1:D:11:GLU:H	1.91	0.78
1:C:51:ALA:HA	3:C:351:HOH:O	1.83	0.78
1:I:202:ARG:NH2	1:I:274:THR:HG23	1.97	0.78
1:G:259:THR:HG21	1:G:266:PRO:HG3	1.66	0.77
1:A:7:GLY:HA2	1:A:33:ALA:O	1.84	0.77
1:H:253:GLU:CD	1:H:253:GLU:H	1.93	0.77
1:C:135:TYR:CE2	1:C:137:PRO:HG3	2.18	0.77
1:I:9:HIS:HB3	1:I:12:ALA:HB3	1.67	0.76
1:D:101:ARG:HD2	1:D:101:ARG:N	1.98	0.76
1:A:146:ILE:HD11	1:A:302:LEU:HD12	1.67	0.76
1:I:72:GLU:HG3	1:I:239:LYS:HD2	1.67	0.76
1:D:259:THR:HG23	1:D:273:SER:HA	1.69	0.75
1:H:93:LYS:HA	3:H:1233:HOH:O	1.86	0.75
1:G:303:LEU:HD12	1:G:309:LYS:HE2	1.68	0.75
1:C:22:ARG:NH2	1:D:186:GLU:HG2	2.02	0.75
1:E:72:GLU:CG	1:E:234:LYS:HA	2.17	0.74
1:G:135:TYR:CE2	1:G:137:PRO:HG3	2.22	0.74
1:D:114:GLU:HA	1:D:117:LEU:HD12	1.69	0.74
1:D:16:VAL:HG11	1:D:249:LEU:CD2	2.17	0.74
1:D:262:ARG:HB3	1:D:264:GLU:OE2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HD11	1:A:188:ASP:HB3	1.68	0.73
1:E:158:ALA:O	1:E:162:LEU:HD13	1.88	0.73
1:H:163:LYS:HD2	3:H:806:HOH:O	1.88	0.73
1:F:278:GLU:HB2	1:F:279:PRO:HD2	1.69	0.73
1:H:187:ILE:HG23	3:H:1274:HOH:O	1.89	0.73
1:C:35:GLY:HA3	3:C:424:HOH:O	1.88	0.73
1:D:101:ARG:HH12	1:D:264:GLU:CB	2.01	0.73
1:D:267:LEU:HD23	1:D:280:ILE:HD13	1.69	0.73
1:D:264:GLU:HG2	3:D:1451:HOH:O	1.88	0.72
1:I:29:LYS:HE3	1:I:31:ASN:HD21	1.54	0.72
1:G:159:LEU:HD23	1:G:302:LEU:HD22	1.72	0.72
1:H:80:ASN:HA	1:H:83:ARG:CD	2.18	0.72
1:E:164:GLY:O	1:E:168:TYR:HD1	1.72	0.72
1:F:183:GLU:C	1:F:184:ASN:OD1	2.33	0.72
1:I:309:LYS:HE3	3:I:841:HOH:O	1.89	0.71
1:A:110:ARG:HE	1:A:210:HIS:CG	2.08	0.71
1:E:43:LYS:HG2	1:E:70:LEU:CD1	2.20	0.71
1:E:36:ASP:O	1:E:39:ALA:HB3	1.90	0.71
1:H:71:LEU:HB2	1:H:94:ASP:HB3	1.72	0.71
1:E:72:GLU:HG2	1:E:234:LYS:CA	2.20	0.71
1:C:80:ASN:HA	1:C:83:ARG:HG3	1.73	0.71
1:I:80:ASN:HB3	1:I:83:ARG:NH2	2.06	0.71
1:I:114:GLU:HA	1:I:117:LEU:HD12	1.72	0.70
1:G:3:THR:OG1	1:G:29:LYS:HE3	1.91	0.70
1:G:252:LYS:H	1:G:252:LYS:HD2	1.56	0.70
1:I:57:GLU:HG2	1:I:58:GLN:HG3	1.73	0.70
1:F:16:VAL:HG11	1:F:249:LEU:HD23	1.72	0.70
1:G:265:TYR:HB3	1:G:280:ILE:CG1	2.21	0.70
1:I:303:LEU:HD13	1:I:309:LYS:HG3	1.74	0.70
1:D:155:GLU:OE2	1:D:298:HIS:HE1	1.75	0.69
1:G:252:LYS:HD2	1:G:252:LYS:N	2.07	0.69
1:E:252:LYS:HE2	1:E:252:LYS:H	1.57	0.69
1:F:265:TYR:CB	1:F:280:ILE:HG12	2.19	0.69
1:E:268:ASN:C	1:E:268:ASN:HD22	2.01	0.69
1:A:224:LEU:HB2	3:A:351:HOH:O	1.93	0.69
1:B:255:GLN:HB2	1:B:271:VAL:HG21	1.73	0.69
1:D:61:ALA:O	1:D:65:LEU:HD22	1.93	0.69
1:A:279:PRO:CD	1:A:282:LYS:HE2	2.17	0.69
1:C:240:ASP:O	1:C:244:LYS:HG3	1.92	0.68
1:C:268:ASN:HD22	1:C:270:HIS:H	1.41	0.68
1:D:197:TRP:HE1	1:D:211:THR:HG23	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:SER:HB2	1:H:94:ASP:HB2	1.75	0.68
1:I:135:TYR:CE2	1:I:137:PRO:HG3	2.28	0.68
1:D:58:GLN:HB2	1:D:60:PRO:HD2	1.76	0.68
1:B:5:TYR:CD1	1:B:51:ALA:HB2	2.28	0.68
1:F:256:ARG:HH22	1:F:272:VAL:H	1.41	0.68
1:D:47:SER:HA	1:D:235:SER:HB2	1.76	0.68
1:H:20:PHE:O	1:H:24:THR:HG23	1.94	0.68
1:I:122:LEU:HA	1:I:161:TRP:CD1	2.29	0.67
1:B:41:GLN:HG2	3:B:550:HOH:O	1.93	0.67
1:H:11:GLU:O	1:H:12:ALA:C	2.38	0.67
1:H:128:LYS:HB3	3:H:1184:HOH:O	1.94	0.67
1:H:4:VAL:HG22	1:H:53:VAL:CB	2.25	0.67
1:A:259:THR:HG21	1:A:266:PRO:HG3	1.77	0.66
1:A:101:ARG:HH22	1:A:228:SER:CB	2.04	0.66
1:D:9:HIS:CG	1:D:11:GLU:OE1	2.49	0.66
1:B:176:SER:O	1:B:180:GLN:HG3	1.94	0.66
1:D:101:ARG:HG3	1:D:101:ARG:HH11	1.60	0.66
1:F:184:ASN:O	1:F:186:GLU:N	2.28	0.66
1:I:255:GLN:HB2	1:I:271:VAL:HG21	1.76	0.66
1:C:204:LYS:HE3	3:C:1506:HOH:O	1.93	0.66
1:A:48:ARG:HA	1:A:48:ARG:NE	2.10	0.66
1:C:265:TYR:CE2	1:C:283:LEU:HD11	2.30	0.66
1:F:248:PHE:O	1:F:254:GLY:HA3	1.95	0.66
1:F:191:LEU:N	1:F:191:LEU:HD22	2.11	0.66
1:D:5:TYR:CE1	1:D:51:ALA:HB2	2.31	0.65
1:B:5:TYR:HA	1:B:31:ASN:HB3	1.79	0.65
1:B:135:TYR:CE2	1:B:137:PRO:HG3	2.31	0.65
1:C:85:LYS:HG3	1:C:86:GLY:H	1.60	0.65
1:D:255:GLN:O	1:D:259:THR:HB	1.97	0.65
1:H:219:ARG:HG3	3:H:1532:HOH:O	1.96	0.65
1:B:237:GLN:H	1:B:237:GLN:CD	2.03	0.65
1:C:301:ARG:HG2	3:C:1111:HOH:O	1.95	0.65
1:I:114:GLU:CD	1:I:214:ASN:HD22	2.04	0.65
1:D:16:VAL:HG11	1:D:249:LEU:HD23	1.79	0.65
1:D:72:GLU:HG3	1:D:239:LYS:HE2	1.77	0.65
1:B:127:PRO:HG3	1:B:168:TYR:CZ	2.31	0.65
1:D:259:THR:CG2	1:D:273:SER:HA	2.27	0.65
1:H:12:ALA:O	1:H:16:VAL:HG23	1.97	0.65
1:B:9:HIS:HD2	1:B:12:ALA:H	1.43	0.64
1:B:197:TRP:CD1	1:B:211:THR:HG22	2.31	0.64
1:E:41:GLN:O	1:E:44:GLU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:HIS:CD2	1:F:11:GLU:HG2	2.32	0.64
1:A:9:HIS:CD2	1:A:11:GLU:H	2.12	0.64
1:C:121:VAL:HG21	1:C:222:GLY:CA	2.20	0.64
1:D:101:ARG:NH1	1:D:264:GLU:HB2	2.12	0.64
1:D:268:ASN:HD22	1:D:270:HIS:H	1.46	0.64
1:A:4:VAL:HG13	1:A:53:VAL:HB	1.79	0.64
1:D:219:ARG:NH1	1:D:285:ALA:O	2.29	0.64
1:H:137:PRO:HB3	1:H:308:MET:HE3	1.79	0.64
1:I:72:GLU:OE1	1:I:73:PRO:HD2	1.98	0.64
1:I:259:THR:HG21	1:I:266:PRO:HG3	1.79	0.64
1:A:57:GLU:HG2	1:A:101:ARG:NH1	2.12	0.64
3:A:1431:HOH:O	1:H:50:PRO:HB3	1.97	0.64
1:D:104:VAL:HG22	1:D:105:VAL:N	2.13	0.64
1:D:111:LYS:O	1:D:112:LEU:HD23	1.97	0.64
1:A:106:VAL:HG22	1:A:213:LEU:CD2	2.28	0.64
1:D:183:GLU:OE1	1:D:211:THR:HG22	1.97	0.64
1:H:236:SER:HB2	1:H:239:LYS:HE2	1.79	0.64
1:G:304:GLU:OE2	1:G:309:LYS:HD3	1.98	0.64
1:D:101:ARG:NH1	1:D:264:GLU:CG	2.55	0.63
1:F:135:TYR:CE2	1:F:137:PRO:HG3	2.33	0.63
1:B:296:LYS:HG2	3:B:1149:HOH:O	1.97	0.63
1:D:5:TYR:CD1	1:D:51:ALA:HB2	2.33	0.63
1:E:4:VAL:HB	1:E:30:LEU:HD23	1.79	0.63
1:H:144:GLU:HG3	1:H:224:LEU:HD21	1.81	0.63
1:B:197:TRP:CD1	1:B:211:THR:CG2	2.82	0.63
1:I:200:PHE:HE1	1:I:204:LYS:HG3	1.59	0.63
1:E:101:ARG:HG3	1:E:101:ARG:HH11	1.63	0.63
1:B:57:GLU:HG2	3:B:320:HOH:O	1.97	0.63
1:F:34:LYS:NZ	1:F:58:GLN:OE1	2.31	0.63
1:F:256:ARG:NH2	1:F:272:VAL:H	1.96	0.63
1:A:48:ARG:HE	1:A:48:ARG:C	2.06	0.62
1:I:129:TRP:O	1:I:130:LYS:C	2.42	0.62
1:B:166:LYS:HD3	1:B:308:MET:HG2	1.81	0.62
1:I:119:LYS:O	1:I:216:VAL:HG23	2.00	0.62
1:I:145:GLN:O	1:I:149:ILE:HG13	2.00	0.62
1:C:5:TYR:CE1	1:C:51:ALA:HB2	2.33	0.62
1:C:80:ASN:OD1	1:C:83:ARG:HD3	1.99	0.62
1:D:297:GLU:O	1:D:301:ARG:HG2	1.98	0.62
1:E:112:LEU:HD12	1:E:116:ASP:HB2	1.80	0.62
1:I:121:VAL:HG13	1:I:122:LEU:HD23	1.81	0.62
1:A:133:ILE:HD11	1:A:191:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ILE:HD12	1:C:93:LYS:HG3	1.82	0.62
1:H:303:LEU:CD1	1:H:309:LYS:HD2	2.29	0.62
1:C:22:ARG:HH22	1:D:186:GLU:HG2	1.65	0.62
1:I:143:LEU:O	1:I:147:VAL:HG23	2.00	0.62
1:F:101:ARG:NH2	1:F:226:THR:HG22	2.15	0.62
1:F:182:VAL:C	1:F:184:ASN:H	2.07	0.62
1:G:4:VAL:HB	1:G:30:LEU:HD23	1.81	0.62
1:H:183:GLU:OE2	1:H:210:HIS:CD2	2.53	0.62
1:D:224:LEU:HD11	3:D:1605:HOH:O	1.98	0.62
1:F:1:ASP:CG	1:F:27:LYS:HB2	2.25	0.62
1:F:129:TRP:CE3	3:F:1325:HOH:O	2.42	0.62
1:F:112:LEU:HD22	3:F:520:HOH:O	1.99	0.62
1:D:118:GLU:HB3	1:D:123:ASN:HB2	1.80	0.62
1:A:219:ARG:N	3:A:1406:HOH:O	2.32	0.62
1:D:217:ARG:NH1	1:D:278:GLU:OE2	2.31	0.62
1:G:53:VAL:HG23	1:G:242:ALA:HB1	1.82	0.62
1:I:108:ASP:HB3	3:I:1227:HOH:O	1.98	0.62
1:G:110:ARG:C	1:G:111:LYS:HD2	2.24	0.61
1:I:9:HIS:HB3	1:I:12:ALA:CB	2.30	0.61
1:I:177:VAL:HG23	3:I:365:HOH:O	1.98	0.61
1:B:36:ASP:OD1	1:B:61:ALA:HB2	2.00	0.61
1:I:81:GLU:OE1	1:I:268:ASN:ND2	2.32	0.61
1:H:17:ALA:HB1	1:H:28:VAL:CG2	2.28	0.61
1:H:66:SER:O	1:H:92:LYS:HE3	2.00	0.61
1:H:245:PHE:O	1:H:249:LEU:HB2	1.99	0.61
1:I:127:PRO:HA	1:I:130:LYS:CG	2.30	0.61
1:B:218:HIS:HA	1:B:284:GLU:OE2	2.00	0.61
1:D:252:LYS:HE3	1:D:252:LYS:H	1.66	0.61
1:F:66:SER:HB2	1:F:71:LEU:HD12	1.82	0.61
1:H:61:ALA:O	1:H:64:THR:HG22	2.01	0.61
1:H:80:ASN:O	1:H:83:ARG:HD3	2.00	0.61
1:I:71:LEU:HB3	1:I:94:ASP:HB2	1.81	0.61
1:E:234:LYS:O	1:E:239:LYS:NZ	2.33	0.61
1:H:8:GLN:HG3	1:H:9:HIS:N	2.14	0.61
1:G:287:GLN:HB2	3:G:1054:HOH:O	2.01	0.61
1:G:303:LEU:HB3	1:G:309:LYS:HE2	1.82	0.61
1:H:53:VAL:HG23	3:H:1069:HOH:O	2.01	0.61
1:A:164:GLY:O	1:A:168:TYR:HD1	1.84	0.61
1:D:267:LEU:CD2	1:D:280:ILE:HD13	2.30	0.60
1:F:184:ASN:C	1:F:186:GLU:H	2.08	0.60
1:G:99:SER:HB2	1:G:264:GLU:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HB2	1:A:115:LYS:HZ2	1.66	0.60
1:G:303:LEU:HB3	1:G:309:LYS:CE	2.30	0.60
1:B:34:LYS:HE3	3:B:1298:HOH:O	2.00	0.60
1:C:236:SER:HB3	1:C:239:LYS:HE2	1.84	0.60
1:D:267:LEU:HD23	1:D:280:ILE:CD1	2.32	0.60
1:G:255:GLN:HE22	1:G:267:LEU:H	1.49	0.60
1:H:279:PRO:HD2	1:H:282:LYS:HG3	1.82	0.60
1:E:66:SER:HB2	1:E:71:LEU:HD12	1.84	0.60
1:I:5:TYR:CE1	1:I:51:ALA:HB2	2.35	0.60
1:I:105:VAL:HG22	1:I:191:LEU:HD23	1.82	0.60
1:I:130:LYS:HA	1:I:168:TYR:O	2.01	0.60
1:C:309:LYS:HB2	3:C:629:HOH:O	2.01	0.60
1:G:142:PHE:O	1:G:146:ILE:HD13	2.02	0.60
1:I:143:LEU:HD21	1:I:296:LYS:HG3	1.84	0.60
1:E:3:THR:HG22	1:E:29:LYS:NZ	2.17	0.60
1:H:76:ALA:HA	1:H:79:ILE:HD12	1.83	0.60
1:I:259:THR:HG22	1:I:266:PRO:HG3	1.84	0.60
1:C:59:ILE:HB	1:C:60:PRO:HD3	1.84	0.60
1:G:99:SER:CB	1:G:264:GLU:HG2	2.32	0.60
1:C:114:GLU:HA	1:C:117:LEU:HD12	1.84	0.59
1:B:239:LYS:HB3	1:B:239:LYS:NZ	2.17	0.59
1:E:43:LYS:HG2	1:E:70:LEU:HD11	1.83	0.59
1:H:62:LEU:HB3	1:H:95:TRP:CD1	2.36	0.59
1:A:117:LEU:HD22	1:A:214:ASN:CB	2.32	0.59
1:F:114:GLU:HG2	1:F:214:ASN:ND2	2.18	0.59
1:I:62:LEU:CD1	1:I:62:LEU:N	2.64	0.59
1:G:20:PHE:HE1	1:G:244:LYS:HG2	1.67	0.59
1:H:34:LYS:HD3	1:H:37:GLN:HE21	1.67	0.59
1:D:110:ARG:HA	3:D:1007:HOH:O	2.03	0.59
1:A:111:LYS:C	1:A:112:LEU:HD23	2.28	0.59
1:C:166:LYS:HE3	1:C:307:GLY:O	2.03	0.59
1:H:162:LEU:HD22	1:H:308:MET:HE1	1.85	0.59
1:H:167:GLU:HG3	1:H:168:TYR:CD2	2.38	0.59
1:I:234:LYS:O	1:I:239:LYS:NZ	2.35	0.59
1:D:239:LYS:O	1:D:243:LYS:HG3	2.03	0.58
1:A:252:LYS:HE2	1:A:256:ARG:NH1	2.14	0.58
1:B:133:ILE:HD11	1:B:191:LEU:HD13	1.85	0.58
1:B:122:LEU:HA	1:B:161:TRP:CD1	2.38	0.58
1:H:62:LEU:HD13	1:H:95:TRP:CB	2.33	0.58
1:I:135:TYR:CD2	1:I:137:PRO:HG3	2.39	0.58
1:A:145:GLN:NE2	3:A:351:HOH:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ALA:HB3	1:E:233:LEU:HD11	1.85	0.58
1:I:72:GLU:HG3	1:I:239:LYS:CD	2.33	0.58
1:B:36:ASP:HB2	3:B:1298:HOH:O	2.03	0.58
1:D:99:SER:OG	1:D:101:ARG:NH2	2.36	0.58
1:F:34:LYS:HD3	1:F:35:GLY:N	2.18	0.58
1:F:166:LYS:HD3	1:F:307:GLY:O	2.04	0.58
1:F:308:MET:O	1:F:308:MET:CG	2.40	0.58
1:A:136:VAL:HG13	1:A:172:TYR:O	2.04	0.58
1:D:7:GLY:HA2	1:D:33:ALA:O	2.02	0.58
1:E:125:ALA:HB1	1:E:164:GLY:HA3	1.85	0.58
1:G:34:LYS:O	1:G:37:GLN:HB3	2.03	0.58
1:A:126:THR:HB	1:A:127:PRO:HD2	1.86	0.58
1:F:136:VAL:O	1:F:139:SER:HB3	2.03	0.58
1:H:38:LEU:HD21	3:H:1604:HOH:O	2.03	0.58
1:H:253:GLU:CD	1:H:253:GLU:N	2.61	0.58
1:A:106:VAL:HG21	1:A:192:ILE:HD11	1.86	0.58
1:A:203:GLU:HG3	1:A:204:LYS:N	2.17	0.58
1:C:120:SER:HB3	1:C:123:ASN:OD1	2.03	0.58
1:D:114:GLU:O	1:D:115:LYS:C	2.45	0.58
1:D:197:TRP:NE1	1:D:211:THR:HG23	2.19	0.58
1:C:81:GLU:OE1	1:C:81:GLU:HA	2.04	0.58
1:D:236:SER:HB3	1:D:239:LYS:HD2	1.85	0.58
1:H:240:ASP:HB2	1:H:243:LYS:HZ1	1.68	0.58
1:H:77:SER:HA	3:H:1079:HOH:O	2.03	0.57
1:H:240:ASP:CB	1:H:243:LYS:HZ1	2.17	0.57
1:I:118:GLU:HB2	1:I:124:TYR:CE2	2.39	0.57
1:A:233:LEU:HD12	1:A:233:LEU:H	1.69	0.57
1:D:72:GLU:HG2	1:D:234:LYS:HA	1.86	0.57
1:E:85:LYS:HD2	1:E:85:LYS:N	2.18	0.57
1:G:6:ASN:O	1:G:32:SER:HA	2.04	0.57
1:H:17:ALA:CB	1:H:28:VAL:HG21	2.28	0.57
1:C:58:GLN:HB2	3:C:424:HOH:O	2.04	0.57
1:F:166:LYS:O	1:F:166:LYS:HE2	2.03	0.57
1:I:54:PHE:CE2	1:I:62:LEU:HD12	2.39	0.57
1:A:48:ARG:NE	1:A:48:ARG:CA	2.67	0.57
1:D:101:ARG:CZ	3:D:1451:HOH:O	2.53	0.57
1:F:81:GLU:HG2	3:F:729:HOH:O	2.04	0.57
1:D:101:ARG:NH1	1:D:101:ARG:HG3	2.20	0.57
1:F:16:VAL:HG11	1:F:249:LEU:CD2	2.34	0.57
1:F:278:GLU:HB2	1:F:279:PRO:CD	2.35	0.57
1:H:54:PHE:HB3	1:H:231:ALA:CB	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:HIS:HA	3:I:1201:HOH:O	2.03	0.57
1:B:106:VAL:CG2	1:B:211:THR:HG23	2.34	0.57
1:D:37:GLN:HG3	3:D:757:HOH:O	2.05	0.57
1:D:256:ARG:HG3	3:D:350:HOH:O	2.04	0.57
1:B:106:VAL:HG23	1:B:211:THR:HG23	1.86	0.57
1:C:303:LEU:HD12	1:C:308:MET:CE	2.31	0.57
1:I:163:LYS:HE2	1:I:306:ALA:HA	1.87	0.57
1:H:273:SER:HA	3:H:1390:HOH:O	2.04	0.56
1:H:216:VAL:HG21	1:H:220:ASP:OD2	2.04	0.56
1:A:110:ARG:NH1	3:A:1141:HOH:O	2.38	0.56
1:B:5:TYR:HB3	1:B:38:LEU:HD13	1.88	0.56
1:D:9:HIS:ND1	1:D:11:GLU:OE1	2.38	0.56
1:F:195:TYR:C	1:F:197:TRP:H	2.13	0.56
1:H:86:GLY:HA2	1:H:287:GLN:NE2	2.21	0.56
1:A:146:ILE:HD12	1:A:158:ALA:HB1	1.87	0.56
1:A:135:TYR:CD2	1:A:137:PRO:HD3	2.40	0.56
1:F:259:THR:HG21	1:F:266:PRO:HG3	1.87	0.56
1:A:130:LYS:O	1:A:132:ARG:HG3	2.06	0.56
1:B:5:TYR:HA	1:B:31:ASN:O	2.05	0.56
1:F:147:VAL:HG13	1:F:295:GLU:CG	2.34	0.56
1:A:300:THR:HG23	1:A:309:LYS:HE3	1.87	0.56
1:D:303:LEU:CD2	1:D:308:MET:HE2	2.35	0.56
1:G:233:LEU:HD12	1:G:233:LEU:N	2.20	0.56
1:C:24:THR:OG1	1:C:26:ILE:HG12	2.05	0.56
1:D:118:GLU:OE2	1:D:129:TRP:NE1	2.28	0.56
1:D:220:ASP:O	1:D:286:PRO:HG3	2.05	0.56
1:D:308:MET:O	1:D:309:LYS:HD2	2.06	0.56
1:F:80:ASN:HD21	1:I:47:SER:CB	2.18	0.56
1:G:282:LYS:HE3	3:G:1294:HOH:O	2.06	0.56
1:H:268:ASN:ND2	3:H:1198:HOH:O	2.39	0.56
1:C:255:GLN:HE22	1:C:267:LEU:H	1.54	0.56
1:D:303:LEU:HD22	1:D:308:MET:HE2	1.88	0.56
1:E:6:ASN:O	1:E:32:SER:HA	2.04	0.56
1:B:178:ALA:O	1:B:182:VAL:HG23	2.06	0.56
1:E:200:PHE:CD1	1:E:200:PHE:N	2.74	0.56
1:C:94:ASP:N	1:C:94:ASP:OD1	2.39	0.55
1:F:108:ASP:C	1:F:108:ASP:OD2	2.49	0.55
1:F:300:THR:HA	1:F:303:LEU:HD12	1.87	0.55
1:H:80:ASN:HB2	3:H:1079:HOH:O	2.06	0.55
1:E:126:THR:HB	1:E:127:PRO:HD2	1.88	0.55
1:E:217:ARG:HH21	1:E:278:GLU:CD	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:ARG:NH2	3:I:774:HOH:O	2.38	0.55
1:A:117:LEU:HD22	1:A:214:ASN:HB2	1.88	0.55
1:E:4:VAL:HB	1:E:30:LEU:CD2	2.36	0.55
1:F:34:LYS:HE2	1:F:57:GLU:OE1	2.06	0.55
1:H:38:LEU:HB2	1:H:54:PHE:HE1	1.70	0.55
1:B:142:PHE:O	1:B:146:ILE:HG13	2.07	0.55
1:E:122:LEU:HA	1:E:161:TRP:CD1	2.42	0.55
1:F:108:ASP:OD2	1:F:110:ARG:HB2	2.07	0.55
1:H:252:LYS:N	3:H:1198:HOH:O	2.25	0.55
1:H:256:ARG:HH11	1:H:256:ARG:HB2	1.70	0.55
1:I:34:LYS:HG3	1:I:37:GLN:HB2	1.87	0.55
1:C:304:GLU:OE2	1:C:309:LYS:HD2	2.05	0.55
1:E:200:PHE:N	1:E:200:PHE:HD1	2.05	0.55
1:I:7:GLY:HA2	1:I:33:ALA:O	2.07	0.55
1:C:46:GLY:O	1:C:47:SER:C	2.50	0.55
1:C:278:GLU:O	1:C:279:PRO:C	2.48	0.55
1:H:2:ILE:HG22	1:H:238:ASN:CB	2.37	0.55
1:I:114:GLU:CD	1:I:214:ASN:ND2	2.63	0.55
1:B:225:VAL:HG23	1:B:285:ALA:HB2	1.88	0.55
1:D:59:ILE:N	1:D:60:PRO:CD	2.70	0.55
1:D:101:ARG:HH12	1:D:264:GLU:HB2	1.67	0.55
1:D:101:ARG:HD2	1:D:226:THR:O	2.07	0.55
1:H:139:SER:HB3	1:H:142:PHE:HB2	1.89	0.55
1:H:272:VAL:C	3:H:1390:HOH:O	2.49	0.55
1:I:65:LEU:HB3	1:I:71:LEU:CD1	2.37	0.55
1:I:100:GLY:O	1:I:264:GLU:HG2	2.05	0.55
1:D:69:ASN:OD1	1:D:92:LYS:NZ	2.37	0.55
1:F:108:ASP:OD1	1:F:185:GLY:HA3	2.07	0.55
1:F:184:ASN:OD1	1:F:184:ASN:N	2.41	0.55
1:G:38:LEU:HD23	1:G:54:PHE:HE1	1.72	0.55
1:E:128:LYS:HZ2	1:E:132:ARG:HH12	1.55	0.54
1:A:211:THR:O	1:A:212:ARG:HD3	2.08	0.54
1:A:256:ARG:HG2	1:A:271:VAL:HG13	1.89	0.54
1:C:48:ARG:HE	1:C:237:GLN:CD	2.16	0.54
1:C:80:ASN:HA	1:C:83:ARG:CG	2.36	0.54
1:D:142:PHE:CE2	1:D:308:MET:HE1	2.42	0.54
1:H:96:VAL:O	1:H:229:GLY:HA2	2.06	0.54
1:I:34:LYS:HG3	1:I:37:GLN:CB	2.36	0.54
1:A:1:ASP:HB3	1:A:26:ILE:HG23	1.88	0.54
1:H:180:GLN:HG3	3:H:1269:HOH:O	2.06	0.54
1:D:34:LYS:HB3	3:D:757:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LEU:HD22	1:D:308:MET:SD	2.47	0.54
1:D:268:ASN:HD22	1:D:268:ASN:C	2.15	0.54
1:I:54:PHE:HE2	1:I:62:LEU:HD12	1.71	0.54
1:B:72:GLU:OE1	1:B:234:LYS:HA	2.07	0.54
1:B:90:ALA:HB2	1:B:95:TRP:CD2	2.43	0.54
1:E:101:ARG:HG3	1:E:101:ARG:NH1	2.22	0.54
1:A:3:THR:HG22	1:A:29:LYS:HB3	1.88	0.54
1:A:239:LYS:O	1:A:243:LYS:HG3	2.07	0.54
1:C:1:ASP:OD2	1:C:27:LYS:HB2	2.08	0.54
1:D:50:PRO:HD3	3:D:338:HOH:O	2.06	0.54
1:F:39:ALA:HA	1:F:42:ILE:HD12	1.89	0.54
1:I:240:ASP:O	1:I:244:LYS:HG2	2.07	0.54
1:B:73:PRO:HG3	3:B:726:HOH:O	2.07	0.54
1:C:308:MET:C	3:C:629:HOH:O	2.50	0.54
1:F:237:GLN:N	1:F:237:GLN:CD	2.66	0.54
1:G:18:ASP:O	1:G:22:ARG:HG3	2.08	0.54
1:H:42:ILE:HD12	1:H:42:ILE:H	1.72	0.54
1:G:193:ASN:HB2	1:G:196:TYR:CE1	2.43	0.54
1:H:24:THR:HG22	1:H:244:LYS:HE2	1.90	0.54
1:G:112:LEU:HD13	1:G:117:LEU:HD21	1.90	0.53
1:G:146:ILE:HG13	1:G:162:LEU:HD21	1.90	0.53
1:A:109:THR:HG21	1:A:212:ARG:HG2	1.90	0.53
1:C:255:GLN:HG3	1:C:268:ASN:HB2	1.91	0.53
1:H:68:ALA:O	1:H:69:ASN:C	2.51	0.53
1:B:2:ILE:HG13	1:B:28:VAL:HG13	1.90	0.53
1:A:115:LYS:HB2	1:A:115:LYS:HZ3	1.72	0.53
1:B:6:ASN:N	1:B:31:ASN:O	2.39	0.53
1:G:209:VAL:HG12	1:G:211:THR:H	1.73	0.53
1:H:2:ILE:HB	3:H:1069:HOH:O	2.08	0.53
1:H:5:TYR:HB3	1:H:38:LEU:HD22	1.91	0.53
1:A:174:LYS:NZ	1:I:23:ALA:O	2.41	0.53
1:A:294:SER:O	1:A:297:GLU:HB3	2.08	0.53
1:D:31:ASN:ND2	3:D:649:HOH:O	2.42	0.53
1:G:54:PHE:CZ	1:G:56:SER:HB2	2.44	0.53
1:B:204:LYS:NZ	3:B:1603:HOH:O	2.41	0.53
1:C:255:GLN:HB3	1:C:271:VAL:HG21	1.91	0.53
1:D:36:ASP:CB	3:D:757:HOH:O	2.56	0.53
1:E:164:GLY:O	1:E:168:TYR:CD1	2.58	0.53
1:G:38:LEU:HD23	1:G:54:PHE:CE1	2.44	0.53
1:H:52:ASP:HB2	3:H:1069:HOH:O	2.08	0.53
1:I:4:VAL:HG22	1:I:53:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLN:HA	1:B:57:GLU:HG3	1.90	0.53
1:C:6:ASN:O	1:C:38:LEU:HD11	2.08	0.53
1:G:151:LYS:HG3	3:G:314:HOH:O	2.08	0.53
1:H:26:ILE:HG12	3:H:1222:HOH:O	2.08	0.53
1:B:42:ILE:O	1:B:45:GLU:HG2	2.09	0.53
1:B:238:ASN:O	1:B:239:LYS:C	2.51	0.53
1:A:9:HIS:HD2	1:A:11:GLU:N	2.01	0.53
1:C:15:ALA:HB2	1:C:261:VAL:HG11	1.91	0.53
1:D:142:PHE:HE2	1:D:308:MET:HE1	1.74	0.53
1:F:9:HIS:CG	1:F:11:GLU:HG2	2.43	0.53
1:F:174:LYS:HD3	1:F:176:SER:OG	2.09	0.53
1:H:136:VAL:HB	1:H:139:SER:HB2	1.91	0.53
1:A:269:PRO:HG2	1:H:48:ARG:HG2	1.91	0.53
1:G:252:LYS:O	1:G:256:ARG:HG3	2.09	0.52
1:H:55:TYR:CE1	1:H:249:LEU:HD21	2.43	0.52
1:I:65:LEU:HB3	1:I:71:LEU:HD11	1.91	0.52
1:D:252:LYS:O	1:D:256:ARG:HB2	2.10	0.52
1:F:133:ILE:N	3:F:1325:HOH:O	2.41	0.52
1:H:71:LEU:HB2	1:H:94:ASP:CB	2.38	0.52
1:D:9:HIS:CD2	1:D:11:GLU:OE2	2.62	0.52
1:D:135:TYR:CE2	1:D:137:PRO:HG3	2.45	0.52
1:D:252:LYS:HD2	1:D:253:GLU:N	2.24	0.52
1:A:218:HIS:CD2	1:A:218:HIS:O	2.62	0.52
1:D:16:VAL:CG1	1:D:248:PHE:HE2	2.23	0.52
1:I:114:GLU:HB2	3:I:862:HOH:O	2.08	0.52
1:B:38:LEU:O	1:B:42:ILE:HG13	2.09	0.52
1:C:101:ARG:HH21	1:C:226:THR:CG2	2.22	0.52
1:C:197:TRP:HE1	1:C:211:THR:HG23	1.74	0.52
1:D:104:VAL:HG23	1:D:214:ASN:O	2.09	0.52
1:E:6:ASN:ND2	1:E:8:GLN:H	2.06	0.52
1:G:100:GLY:O	1:G:264:GLU:HG3	2.09	0.52
1:G:121:VAL:CG1	1:G:222:GLY:HA3	2.40	0.52
1:I:185:GLY:HA2	3:I:1232:HOH:O	2.08	0.52
1:A:3:THR:HG22	1:A:29:LYS:HG2	1.91	0.52
1:A:16:VAL:HG11	1:A:249:LEU:CD2	2.40	0.52
1:A:113:SER:O	1:A:117:LEU:HD12	2.09	0.52
1:C:41:GLN:HA	1:C:44:GLU:HB2	1.91	0.52
1:F:179:LEU:HD22	1:F:196:TYR:O	2.09	0.52
1:H:93:LYS:HD2	1:H:93:LYS:N	2.25	0.52
1:B:9:HIS:CD2	1:B:12:ALA:H	2.27	0.52
1:D:101:ARG:NH1	3:D:1451:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:ARG:CG	1:E:264:GLU:HG3	2.35	0.52
1:F:255:GLN:HB2	1:F:271:VAL:HG21	1.91	0.52
1:I:111:LYS:HB2	3:I:1227:HOH:O	2.10	0.52
1:I:182:VAL:HG13	1:I:211:THR:CG2	2.35	0.52
1:A:43:LYS:HG3	3:A:1402:HOH:O	2.08	0.52
1:A:233:LEU:HD12	1:A:233:LEU:N	2.24	0.52
1:E:44:GLU:O	1:E:45:GLU:C	2.52	0.52
1:E:99:SER:HA	1:E:267:LEU:HG	1.90	0.52
1:G:99:SER:OG	1:G:264:GLU:HG2	2.10	0.52
1:G:140:GLY:O	1:G:144:GLU:HG2	2.10	0.52
1:H:126:THR:HB	1:H:127:PRO:CD	2.39	0.52
1:B:99:SER:HA	1:B:267:LEU:HG	1.92	0.52
1:C:197:TRP:HB3	1:C:213:LEU:HD11	1.91	0.52
1:C:197:TRP:NE1	1:C:211:THR:HG23	2.25	0.51
1:G:234:LYS:HB2	3:G:706:HOH:O	2.09	0.51
1:I:6:ASN:HD21	1:I:8:GLN:HB3	1.74	0.51
1:B:46:GLY:O	1:B:235:SER:HB3	2.09	0.51
1:B:114:GLU:HA	1:B:117:LEU:HD12	1.92	0.51
1:I:258:LEU:C	1:I:260:ALA:H	2.18	0.51
1:C:79:ILE:O	1:C:83:ARG:HG3	2.10	0.51
1:I:143:LEU:HB3	3:I:1112:HOH:O	2.10	0.51
1:B:67:ALA:C	1:B:69:ASN:H	2.18	0.51
1:C:142:PHE:O	1:C:146:ILE:HG13	2.11	0.51
1:E:92:LYS:HB2	1:E:94:ASP:CG	2.35	0.51
1:G:90:ALA:HB2	1:G:95:TRP:CE2	2.46	0.51
1:I:43:LYS:HZ2	1:I:68:ALA:HB1	1.76	0.51
1:I:62:LEU:HD13	1:I:62:LEU:H	1.75	0.51
1:I:181:ALA:O	1:I:186:GLU:HB2	2.10	0.51
1:G:218:HIS:N	1:G:284:GLU:OE2	2.43	0.51
1:A:43:LYS:HE3	3:A:1402:HOH:O	2.10	0.51
1:A:272:VAL:HG22	1:A:272:VAL:O	2.09	0.51
1:D:198:HIS:CD2	3:D:1446:HOH:O	2.64	0.51
1:F:192:ILE:CG2	1:F:193:ASN:N	2.54	0.51
1:H:130:LYS:HE3	3:H:500:HOH:O	2.10	0.51
1:D:2:ILE:O	1:D:2:ILE:HG13	2.11	0.51
1:F:113:SER:OG	1:F:115:LYS:HG2	2.10	0.51
1:H:2:ILE:HG23	1:H:241:GLU:HB3	1.93	0.51
1:A:106:VAL:HG22	1:A:213:LEU:HD23	1.92	0.51
1:A:110:ARG:HE	1:A:210:HIS:CD2	2.29	0.51
1:H:55:TYR:CD1	1:H:249:LEU:HD21	2.45	0.51
1:H:256:ARG:HB2	1:H:256:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:ARG:HB3	1:I:188:ASP:HB2	1.92	0.51
1:C:255:GLN:HE22	1:C:267:LEU:N	2.09	0.51
1:D:135:TYR:O	1:D:137:PRO:HD3	2.11	0.51
1:H:43:LYS:NZ	1:H:65:LEU:HD23	2.25	0.51
1:C:114:GLU:C	1:C:115:LYS:HD2	2.37	0.50
1:D:9:HIS:CE1	1:D:11:GLU:OE2	2.63	0.50
1:E:300:THR:O	1:E:303:LEU:HB2	2.11	0.50
1:G:3:THR:HG23	1:G:29:LYS:HD2	1.93	0.50
1:A:3:THR:HG21	1:A:29:LYS:NZ	2.25	0.50
1:D:204:LYS:HD3	1:D:204:LYS:N	2.26	0.50
1:D:256:ARG:CZ	1:D:256:ARG:HB3	2.42	0.50
1:E:6:ASN:HD21	1:E:8:GLN:HB2	1.76	0.50
1:F:107:TYR:CE2	1:F:109:THR:HG22	2.46	0.50
1:H:42:ILE:HG21	1:H:233:LEU:HD12	1.94	0.50
1:H:304:GLU:HG3	1:H:309:LYS:HB2	1.92	0.50
1:F:34:LYS:HD3	1:F:34:LYS:C	2.36	0.50
1:F:298:HIS:O	1:F:302:LEU:HG	2.12	0.50
1:H:74:LEU:HB2	1:H:93:LYS:O	2.11	0.50
1:I:43:LYS:NZ	1:I:68:ALA:HB1	2.26	0.50
1:F:115:LYS:C	1:F:117:LEU:H	2.20	0.50
1:G:163:LYS:HD2	1:G:306:ALA:HA	1.94	0.50
1:G:185:GLY:HA2	3:G:1285:HOH:O	2.12	0.50
1:H:80:ASN:CB	3:H:1079:HOH:O	2.60	0.50
1:H:176:SER:O	1:H:180:GLN:NE2	2.44	0.50
1:B:133:ILE:N	1:B:187:ILE:HD11	2.27	0.50
1:C:255:GLN:O	1:C:259:THR:HG22	2.12	0.50
1:B:175:ASN:HD22	1:B:192:ILE:HG22	1.76	0.50
1:C:256:ARG:HA	1:C:259:THR:HG22	1.94	0.50
1:H:42:ILE:HG12	1:H:233:LEU:HD11	1.92	0.50
1:H:135:TYR:CE2	1:H:308:MET:HE3	2.46	0.50
1:C:93:LYS:O	1:C:93:LYS:HG2	2.11	0.50
1:F:217:ARG:NH1	1:F:278:GLU:OE2	2.45	0.50
1:I:79:ILE:O	1:I:83:ARG:HB3	2.11	0.50
1:A:142:PHE:O	1:A:146:ILE:HG22	2.12	0.50
1:B:283:LEU:O	1:B:284:GLU:HB2	2.12	0.50
1:C:292:THR:OG1	1:C:295:GLU:HG3	2.12	0.50
1:E:209:VAL:HG12	1:E:211:THR:H	1.77	0.50
1:H:121:VAL:HA	1:H:124:TYR:HD2	1.76	0.50
1:I:255:GLN:CB	1:I:271:VAL:HG21	2.42	0.50
1:B:170:LYS:HE2	1:B:187:ILE:HD12	1.94	0.50
1:D:155:GLU:O	1:D:156:ALA:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:LYS:HB2	1:G:177:VAL:HG23	1.94	0.50
1:H:83:ARG:N	1:H:83:ARG:HD2	2.26	0.50
1:I:80:ASN:HA	1:I:83:ARG:HB3	1.93	0.50
1:A:74:LEU:HB2	1:A:79:ILE:HD11	1.93	0.49
1:A:164:GLY:O	1:A:168:TYR:CD1	2.65	0.49
1:H:2:ILE:HD13	1:H:26:ILE:CG2	2.41	0.49
1:H:28:VAL:HG22	3:H:1139:HOH:O	2.11	0.49
1:H:64:THR:HG23	1:H:65:LEU:HG	1.94	0.49
1:H:194:ASN:CG	1:H:195:TYR:N	2.70	0.49
1:H:300:THR:O	1:H:303:LEU:HB2	2.12	0.49
1:I:44:GLU:HG3	1:I:45:GLU:N	2.27	0.49
1:I:117:LEU:HD13	1:I:214:ASN:HB2	1.93	0.49
1:B:80:ASN:HB3	3:G:1158:HOH:O	2.12	0.49
1:F:237:GLN:CD	1:F:237:GLN:H	2.18	0.49
1:G:256:ARG:HG2	1:G:271:VAL:HG13	1.94	0.49
1:H:71:LEU:HB2	1:H:94:ASP:CG	2.37	0.49
1:A:216:VAL:HG22	3:A:316:HOH:O	2.13	0.49
1:D:118:GLU:CB	1:D:123:ASN:HB2	2.41	0.49
1:F:115:LYS:O	1:F:116:ASP:CG	2.55	0.49
1:F:135:TYR:CD2	1:F:137:PRO:HG3	2.47	0.49
1:F:214:ASN:HB3	3:F:347:HOH:O	2.12	0.49
1:B:107:TYR:HB2	1:B:112:LEU:HD11	1.94	0.49
1:C:197:TRP:CD1	1:C:211:THR:HG23	2.48	0.49
1:D:56:SER:O	1:D:228:SER:HB3	2.13	0.49
1:H:5:TYR:OH	1:H:50:PRO:HD2	2.13	0.49
1:A:148:ALA:HB3	3:A:351:HOH:O	2.11	0.49
1:C:135:TYR:HE2	1:C:137:PRO:HG3	1.74	0.49
1:G:255:GLN:NE2	1:G:268:ASN:H	2.10	0.49
1:I:80:ASN:HB3	1:I:83:ARG:CZ	2.42	0.49
1:A:12:ALA:O	1:A:16:VAL:HG23	2.12	0.49
1:C:252:LYS:HE2	1:C:270:HIS:CB	2.41	0.49
1:G:137:PRO:O	1:G:138:THR:HG23	2.12	0.49
1:I:108:ASP:C	1:I:110:ARG:H	2.20	0.49
1:A:59:ILE:N	1:A:60:PRO:CD	2.76	0.49
1:B:17:ALA:HB1	3:B:1209:HOH:O	2.11	0.49
1:C:159:LEU:HG	1:C:163:LYS:HE3	1.95	0.49
1:D:34:LYS:HB3	1:D:37:GLN:HG3	1.94	0.49
1:G:265:TYR:HB3	1:G:280:ILE:HG12	1.95	0.49
1:H:57:GLU:OE2	1:H:57:GLU:N	2.35	0.49
1:I:77:SER:O	1:I:80:ASN:ND2	2.46	0.49
1:B:32:SER:O	1:B:33:ALA:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:THR:HA	1:D:112:LEU:O	2.13	0.49
1:D:303:LEU:HB3	1:D:309:LYS:HB2	1.95	0.49
1:H:28:VAL:HB	3:H:425:HOH:O	2.12	0.49
1:H:199:ALA:O	1:H:203:GLU:HG3	2.13	0.49
1:A:9:HIS:O	1:A:12:ALA:HB3	2.12	0.49
1:A:18:ASP:O	1:A:22:ARG:HG3	2.13	0.49
1:C:233:LEU:N	1:C:233:LEU:HD12	2.28	0.49
1:D:155:GLU:OE2	1:D:298:HIS:CE1	2.59	0.49
1:I:81:GLU:OE1	1:I:251:GLY:HA2	2.13	0.49
1:F:256:ARG:HH22	1:F:272:VAL:N	2.08	0.49
1:I:130:LYS:HG2	1:I:168:TYR:HB3	1.93	0.49
1:C:5:TYR:CD1	1:C:51:ALA:HB2	2.47	0.48
1:D:81:GLU:HB2	1:D:250:ALA:HB1	1.95	0.48
1:D:114:GLU:HA	1:D:117:LEU:CD1	2.41	0.48
1:D:155:GLU:O	1:D:158:ALA:N	2.46	0.48
1:F:275:PHE:CD1	3:F:1091:HOH:O	2.47	0.48
1:I:257:ALA:O	1:I:260:ALA:HB3	2.13	0.48
1:D:245:PHE:O	1:D:248:PHE:HB3	2.12	0.48
1:F:136:VAL:HG11	1:F:174:LYS:HA	1.95	0.48
1:G:265:TYR:HB3	1:G:280:ILE:HG13	1.95	0.48
1:I:265:TYR:CD1	1:I:265:TYR:N	2.81	0.48
1:E:135:TYR:O	1:E:171:PRO:HA	2.12	0.48
1:G:303:LEU:HD13	1:G:308:MET:HB2	1.94	0.48
1:B:41:GLN:O	1:B:44:GLU:HG2	2.14	0.48
1:A:8:GLN:NE2	1:A:55:TYR:CE1	2.81	0.48
1:H:2:ILE:HG22	1:H:238:ASN:HB2	1.94	0.48
1:H:257:ALA:O	1:H:260:ALA:HB3	2.13	0.48
1:I:209:VAL:O	1:I:212:ARG:NH2	2.46	0.48
1:A:110:ARG:NE	1:A:210:HIS:CG	2.80	0.48
1:D:106:VAL:HG22	1:D:211:THR:OG1	2.13	0.48
1:D:256:ARG:HB3	1:D:256:ARG:NH1	2.28	0.48
1:E:8:GLN:NE2	1:E:228:SER:HB3	2.29	0.48
1:G:24:THR:CG2	1:G:244:LYS:HE2	2.44	0.48
1:H:38:LEU:HD11	3:H:1604:HOH:O	2.14	0.48
1:I:220:ASP:CG	1:I:221:PRO:HD2	2.38	0.48
1:F:118:GLU:HB2	1:F:124:TYR:CZ	2.49	0.48
1:A:122:LEU:HA	1:A:161:TRP:CD1	2.48	0.48
1:B:34:LYS:HB2	3:B:1298:HOH:O	2.13	0.48
1:B:252:LYS:HE3	1:B:270:HIS:O	2.14	0.48
1:C:17:ALA:O	1:C:20:PHE:HB3	2.14	0.48
1:D:265:TYR:N	1:D:265:TYR:CD1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:VAL:HG22	1:G:187:ILE:HG23	1.95	0.48
1:H:303:LEU:HB3	1:H:309:LYS:CG	2.33	0.48
1:B:69:ASN:OD1	1:B:92:LYS:HE2	2.13	0.48
1:C:80:ASN:HA	1:C:83:ARG:CD	2.44	0.48
1:E:84:GLY:HA2	3:E:551:HOH:O	2.14	0.48
1:F:108:ASP:OD2	1:F:110:ARG:N	2.47	0.48
1:G:18:ASP:N	1:G:18:ASP:OD1	2.45	0.48
1:H:121:VAL:HA	1:H:124:TYR:CD2	2.48	0.48
1:H:173:ALA:N	3:H:578:HOH:O	2.42	0.48
1:A:33:ALA:HB3	1:A:38:LEU:HG	1.96	0.48
1:A:108:ASP:OD2	1:A:110:ARG:HG3	2.13	0.48
1:A:218:HIS:O	1:A:218:HIS:HD2	1.97	0.48
1:B:3:THR:HG23	1:B:29:LYS:HE3	1.95	0.48
1:E:233:LEU:HD12	1:E:235:SER:OG	2.14	0.48
1:H:11:GLU:O	1:H:14:GLN:N	2.46	0.48
1:H:136:VAL:C	1:H:138:THR:H	2.21	0.48
1:B:72:GLU:CA	1:B:234:LYS:HG3	2.44	0.47
1:C:183:GLU:HG3	3:C:1146:HOH:O	2.14	0.47
1:D:220:ASP:CG	1:D:221:PRO:HD2	2.38	0.47
1:F:184:ASN:HB2	1:F:186:GLU:HG2	1.95	0.47
1:H:72:GLU:HA	1:H:73:PRO:HD3	1.75	0.47
1:I:62:LEU:N	1:I:62:LEU:HD12	2.29	0.47
1:B:136:VAL:CG1	1:B:139:SER:HB3	2.44	0.47
1:B:239:LYS:HE2	1:B:243:LYS:HZ2	1.79	0.47
1:C:197:TRP:HE1	1:C:211:THR:CG2	2.28	0.47
1:E:128:LYS:NZ	1:E:132:ARG:HH12	2.12	0.47
1:H:178:ALA:O	1:H:182:VAL:HG23	2.13	0.47
1:H:200:PHE:CE1	1:H:204:LYS:HG3	2.49	0.47
1:C:255:GLN:NE2	1:C:268:ASN:H	2.11	0.47
1:E:130:LYS:O	1:E:132:ARG:HG3	2.15	0.47
1:E:268:ASN:HD22	1:E:270:HIS:H	1.62	0.47
1:F:255:GLN:NE2	1:F:268:ASN:H	2.13	0.47
1:G:100:GLY:HA2	1:G:226:THR:O	2.14	0.47
1:H:135:TYR:HD2	1:H:142:PHE:CZ	2.32	0.47
1:A:126:THR:HB	1:A:127:PRO:CD	2.44	0.47
1:C:239:LYS:HB2	1:C:239:LYS:HE3	1.62	0.47
1:F:107:TYR:O	1:F:211:THR:HA	2.14	0.47
1:F:146:ILE:O	1:F:150:VAL:HG23	2.15	0.47
1:G:14:GLN:O	1:G:18:ASP:OD1	2.31	0.47
1:H:76:ALA:O	1:H:80:ASN:HB2	2.14	0.47
1:I:92:LYS:HE3	3:I:354:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:PRO:HA	1:B:94:ASP:HA	1.95	0.47
1:F:103:ARG:HD3	3:F:316:HOH:O	2.15	0.47
1:F:184:ASN:C	1:F:186:GLU:N	2.72	0.47
1:I:20:PHE:O	1:I:23:ALA:HB3	2.15	0.47
1:I:82:THR:HB	1:I:267:LEU:CB	2.38	0.47
1:B:252:LYS:HG2	1:B:256:ARG:CZ	2.45	0.47
1:E:200:PHE:HD1	1:E:200:PHE:H	1.63	0.47
1:F:236:SER:HB3	1:F:239:LYS:HG3	1.97	0.47
1:F:237:GLN:H	1:F:237:GLN:NE2	2.12	0.47
1:G:265:TYR:CE2	1:G:283:LEU:HD11	2.49	0.47
1:I:9:HIS:O	1:I:13:ALA:N	2.44	0.47
1:A:1:ASP:CB	1:A:26:ILE:HG23	2.45	0.47
1:A:130:LYS:HG3	3:A:1610:HOH:O	2.15	0.47
1:B:57:GLU:O	1:B:101:ARG:NH2	2.46	0.47
1:D:2:ILE:HA	1:D:52:ASP:OD1	2.15	0.47
1:D:239:LYS:O	1:D:240:ASP:C	2.57	0.47
1:E:101:ARG:HH11	1:E:101:ARG:CG	2.23	0.47
1:E:268:ASN:ND2	1:E:270:HIS:H	2.13	0.47
1:F:45:GLU:OE1	1:F:50:PRO:HD2	2.14	0.47
1:F:174:LYS:HG3	1:F:177:VAL:HG23	1.97	0.47
1:I:10:LYS:HE3	1:I:32:SER:HB2	1.97	0.47
1:D:101:ARG:NE	1:D:228:SER:OG	2.39	0.47
1:F:118:GLU:HB2	1:F:124:TYR:CE2	2.50	0.47
1:F:217:ARG:HB3	1:F:284:GLU:OE2	2.15	0.47
1:G:101:ARG:HD2	1:G:195:TYR:CE1	2.50	0.47
1:H:19:ALA:HB1	1:H:248:PHE:HZ	1.80	0.47
1:I:34:LYS:HE2	1:I:37:GLN:OE1	2.15	0.47
1:I:110:ARG:HH11	1:I:210:HIS:CG	2.33	0.47
1:I:155:GLU:OE1	1:I:298:HIS:HE1	1.98	0.47
1:I:216:VAL:O	1:I:218:HIS:HD2	1.96	0.47
1:A:1:ASP:OD2	1:A:27:LYS:HB2	2.14	0.47
1:B:237:GLN:OE1	1:B:237:GLN:N	2.46	0.47
1:D:43:LYS:HE3	1:D:64:THR:HG22	1.97	0.47
1:F:182:VAL:C	1:F:184:ASN:N	2.70	0.47
1:B:136:VAL:HG12	1:B:139:SER:HB3	1.97	0.47
1:F:4:VAL:HG22	1:F:53:VAL:HB	1.97	0.47
1:H:4:VAL:HG23	3:H:425:HOH:O	2.15	0.47
1:H:167:GLU:HG3	1:H:168:TYR:CE2	2.50	0.47
1:H:252:LYS:HA	1:H:255:GLN:HB2	1.97	0.47
1:H:265:TYR:CZ	1:H:277:LEU:HD22	2.49	0.47
1:A:9:HIS:CD2	1:A:11:GLU:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:VAL:HG13	1:D:151:LYS:HE3	1.97	0.46
1:D:303:LEU:HD13	1:D:309:LYS:HE3	1.96	0.46
1:E:130:LYS:HD2	1:E:131:ASN:N	2.29	0.46
1:G:101:ARG:HD3	1:G:262:ARG:NH2	2.29	0.46
1:B:54:PHE:O	1:B:230:ALA:HA	2.15	0.46
1:D:103:ARG:HH21	1:D:193:ASN:ND2	2.12	0.46
1:F:195:TYR:C	1:F:197:TRP:N	2.73	0.46
1:G:99:SER:HB2	1:G:265:TYR:O	2.15	0.46
1:H:71:LEU:CB	1:H:94:ASP:HB3	2.43	0.46
1:B:72:GLU:HB2	1:B:234:LYS:HA	1.96	0.46
1:B:259:THR:HG23	1:B:273:SER:HA	1.97	0.46
1:D:36:ASP:HB3	3:D:757:HOH:O	2.14	0.46
1:G:58:GLN:HG2	1:G:60:PRO:HD2	1.96	0.46
1:I:110:ARG:HH22	1:I:185:GLY:CA	2.29	0.46
1:A:278:GLU:HB3	1:A:282:LYS:HE3	1.93	0.46
1:F:11:GLU:HG3	1:F:12:ALA:N	2.30	0.46
1:G:76:ALA:O	1:G:77:SER:C	2.58	0.46
1:G:202:ARG:HH22	1:G:274:THR:CG2	2.21	0.46
1:G:220:ASP:OD1	1:G:221:PRO:HD2	2.15	0.46
1:I:103:ARG:NH2	1:I:192:ILE:HA	2.31	0.46
1:I:265:TYR:HA	1:I:266:PRO:HD3	1.66	0.46
1:A:252:LYS:HD2	1:H:237:GLN:CD	2.41	0.46
1:C:22:ARG:HH22	1:D:186:GLU:CG	2.28	0.46
1:F:45:GLU:HB3	1:F:49:SER:HA	1.96	0.46
1:G:121:VAL:HG11	1:G:222:GLY:HA3	1.97	0.46
1:H:126:THR:HB	1:H:127:PRO:HD2	1.97	0.46
1:I:183:GLU:OE1	1:I:209:VAL:HA	2.16	0.46
1:C:101:ARG:NH2	1:C:226:THR:CG2	2.78	0.46
1:C:278:GLU:O	1:C:278:GLU:HG2	2.15	0.46
1:D:267:LEU:HA	1:D:280:ILE:CD1	2.37	0.46
1:E:85:LYS:HD2	1:E:85:LYS:H	1.80	0.46
1:H:20:PHE:CD2	1:H:245:PHE:HD1	2.34	0.46
1:E:244:LYS:HD2	3:E:1109:HOH:O	2.14	0.46
1:G:79:ILE:C	3:G:1518:HOH:O	2.59	0.46
1:G:126:THR:HA	1:G:168:TYR:CE1	2.51	0.46
1:G:135:TYR:CD2	1:G:137:PRO:HG3	2.51	0.46
1:H:85:LYS:C	1:H:87:VAL:H	2.24	0.46
1:I:161:TRP:CZ2	1:I:165:LEU:HD11	2.51	0.46
1:I:175:ASN:OD1	1:I:196:TYR:CE1	2.69	0.46
1:D:170:LYS:HD2	1:D:187:ILE:HD12	1.98	0.46
1:E:268:ASN:C	1:E:268:ASN:ND2	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:ILE:HD13	1:H:26:ILE:HG22	1.98	0.46
1:I:8:GLN:HE21	1:I:8:GLN:HB2	1.58	0.46
1:I:255:GLN:O	1:I:258:LEU:HB3	2.16	0.46
1:A:167:GLU:HG2	1:A:168:TYR:CZ	2.52	0.46
1:F:57:GLU:O	1:F:101:ARG:NH2	2.49	0.46
1:G:239:LYS:O	1:G:243:LYS:HG3	2.16	0.46
1:I:21:THR:C	1:I:23:ALA:H	2.23	0.46
1:I:72:GLU:HG2	1:I:234:LYS:HA	1.97	0.46
1:B:40:GLY:O	1:B:41:GLN:C	2.59	0.45
1:B:255:GLN:O	1:B:259:THR:HB	2.16	0.45
1:C:25:GLY:HA3	3:C:439:HOH:O	2.15	0.45
1:C:173:ALA:O	1:C:174:LYS:HG2	2.17	0.45
1:H:240:ASP:HA	1:H:243:LYS:HB2	1.98	0.45
1:I:258:LEU:C	1:I:260:ALA:N	2.73	0.45
1:A:174:LYS:HA	1:A:174:LYS:HD3	1.69	0.45
1:B:251:GLY:O	1:B:252:LYS:C	2.59	0.45
1:C:265:TYR:HA	1:C:266:PRO:HD3	1.82	0.45
1:G:248:PHE:O	1:G:254:GLY:HA3	2.16	0.45
1:G:255:GLN:HB2	1:G:271:VAL:HG21	1.98	0.45
1:A:40:GLY:O	1:A:44:GLU:HG2	2.16	0.45
1:B:59:ILE:HB	1:B:60:PRO:HD3	1.97	0.45
1:D:58:GLN:HA	3:D:319:HOH:O	2.16	0.45
1:A:219:ARG:HG2	3:A:1406:HOH:O	2.17	0.45
1:D:100:GLY:O	1:D:264:GLU:CB	2.64	0.45
1:D:144:GLU:CG	1:D:224:LEU:HD21	2.46	0.45
1:E:301:ARG:HA	1:E:301:ARG:HD3	1.50	0.45
1:H:117:LEU:HD12	1:H:124:TYR:OH	2.15	0.45
1:H:135:TYR:HE2	1:H:308:MET:CE	2.30	0.45
1:I:8:GLN:NE2	1:I:55:TYR:CE1	2.83	0.45
1:B:198:HIS:HE1	3:B:1444:HOH:O	1.98	0.45
1:D:203:GLU:HG3	1:D:204:LYS:HD3	1.99	0.45
1:G:122:LEU:HA	1:G:161:TRP:CD1	2.52	0.45
1:I:2:ILE:HG22	1:I:238:ASN:HB2	1.99	0.45
1:A:106:VAL:HG21	1:A:192:ILE:CD1	2.46	0.45
1:C:218:HIS:HA	1:C:284:GLU:OE2	2.16	0.45
1:E:49:SER:HA	1:E:50:PRO:HD3	1.85	0.45
1:E:170:LYS:CD	1:E:187:ILE:HD12	2.31	0.45
1:E:255:GLN:O	1:E:259:THR:HG22	2.16	0.45
1:G:72:GLU:OE1	1:G:234:LYS:HA	2.16	0.45
1:B:9:HIS:CD2	1:B:11:GLU:HB2	2.52	0.45
1:B:34:LYS:O	1:B:38:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ASN:ND2	1:C:270:HIS:H	2.12	0.45
1:E:253:GLU:CD	1:E:253:GLU:H	2.25	0.45
1:H:95:TRP:O	1:H:95:TRP:CE3	2.70	0.45
1:A:80:ASN:CG	1:A:83:ARG:HH21	2.25	0.45
1:C:85:LYS:HG3	1:C:86:GLY:N	2.30	0.45
1:C:113:SER:O	1:C:115:LYS:N	2.41	0.45
1:F:33:ALA:HB3	1:F:38:LEU:HD13	1.97	0.45
1:F:109:THR:HG21	1:F:212:ARG:HG2	1.99	0.45
1:C:255:GLN:CB	1:C:271:VAL:HG21	2.47	0.45
1:F:206:VAL:HG22	1:F:212:ARG:NH2	2.32	0.45
1:A:51:ALA:HB3	1:A:233:LEU:HD22	1.97	0.45
1:A:112:LEU:CD1	1:A:188:ASP:HB3	2.43	0.45
1:G:79:ILE:HG22	1:G:83:ARG:NH1	2.32	0.45
1:I:49:SER:HA	1:I:50:PRO:HD3	1.83	0.45
1:A:83:ARG:HG3	3:A:1125:HOH:O	2.17	0.44
1:A:110:ARG:CZ	3:A:1141:HOH:O	2.65	0.44
1:B:38:LEU:HB2	1:B:54:PHE:CE1	2.52	0.44
1:B:59:ILE:HD11	1:B:227:TYR:HB2	1.98	0.44
1:B:248:PHE:O	1:B:254:GLY:HA3	2.17	0.44
1:C:244:LYS:O	1:C:247:ALA:HB3	2.17	0.44
1:D:24:THR:HB	1:D:26:ILE:HD12	1.98	0.44
1:D:114:GLU:O	1:D:116:ASP:N	2.51	0.44
1:D:139:SER:HB3	1:D:142:PHE:HB2	1.99	0.44
1:D:217:ARG:HG2	1:D:217:ARG:HH11	1.82	0.44
1:E:54:PHE:CZ	1:E:56:SER:HB3	2.51	0.44
1:G:110:ARG:O	1:G:111:LYS:HD2	2.17	0.44
1:H:172:TYR:CB	1:H:178:ALA:HB2	2.47	0.44
1:I:57:GLU:OE1	1:I:58:GLN:NE2	2.50	0.44
1:I:119:LYS:O	1:I:216:VAL:CG2	2.64	0.44
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.80	0.44
1:F:133:ILE:CB	3:F:1325:HOH:O	2.43	0.44
1:H:197:TRP:CB	1:H:213:LEU:HD21	2.48	0.44
1:I:259:THR:HG21	1:I:266:PRO:CG	2.46	0.44
1:C:101:ARG:HH21	1:C:226:THR:HG22	1.81	0.44
1:E:112:LEU:HD12	1:E:116:ASP:CB	2.47	0.44
1:E:255:GLN:HB2	1:E:271:VAL:HG21	1.99	0.44
1:G:176:SER:O	1:G:180:GLN:HG2	2.18	0.44
1:H:121:VAL:HG12	1:H:124:TYR:CE2	2.52	0.44
1:H:159:LEU:HD12	1:H:159:LEU:O	2.17	0.44
1:H:175:ASN:HD22	1:H:192:ILE:HG22	1.83	0.44
1:H:248:PHE:O	1:H:254:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ILE:HD13	1:A:233:LEU:HD21	1.98	0.44
1:D:101:ARG:HD2	1:D:101:ARG:H	1.82	0.44
1:D:280:ILE:H	1:D:280:ILE:HG13	1.50	0.44
1:E:297:GLU:OE1	1:E:297:GLU:HA	2.17	0.44
1:F:145:GLN:HA	1:F:145:GLN:NE2	2.33	0.44
1:G:220:ASP:CG	1:G:221:PRO:HD2	2.43	0.44
1:B:111:LYS:HA	1:B:111:LYS:HD2	1.64	0.44
1:E:20:PHE:CD2	1:E:245:PHE:HD1	2.35	0.44
1:F:179:LEU:CD2	1:F:196:TYR:O	2.66	0.44
1:F:256:ARG:NH1	1:F:272:VAL:O	2.45	0.44
1:H:2:ILE:HG22	1:H:238:ASN:HB3	1.98	0.44
1:I:54:PHE:CE2	1:I:62:LEU:CD1	3.00	0.44
1:A:105:VAL:HB	1:A:214:ASN:HB3	1.99	0.44
1:B:72:GLU:N	1:B:234:LYS:HG3	2.33	0.44
1:D:239:LYS:HB3	1:D:243:LYS:HE3	1.99	0.44
1:F:110:ARG:NH2	1:F:183:GLU:C	2.63	0.44
1:F:143:LEU:O	1:F:146:ILE:HB	2.17	0.44
1:G:202:ARG:CZ	1:G:274:THR:HG22	2.46	0.44
1:H:219:ARG:HD3	1:H:284:GLU:O	2.17	0.44
1:I:126:THR:HB	1:I:127:PRO:HD2	2.00	0.44
1:B:71:LEU:CB	1:B:94:ASP:HB2	2.48	0.44
1:B:259:THR:CG2	1:B:273:SER:HA	2.48	0.44
1:C:78:THR:O	1:C:81:GLU:HB2	2.16	0.44
1:C:248:PHE:CE2	1:C:254:GLY:HA2	2.53	0.44
1:E:59:ILE:N	1:E:60:PRO:CD	2.81	0.44
1:F:72:GLU:OE1	1:F:239:LYS:NZ	2.46	0.44
1:F:132:ARG:C	3:F:1325:HOH:O	2.60	0.44
1:G:125:ALA:HB1	1:G:164:GLY:HA3	1.99	0.44
1:H:139:SER:HB3	1:H:142:PHE:CB	2.48	0.44
1:I:256:ARG:HA	1:I:259:THR:OG1	2.17	0.44
1:A:34:LYS:O	1:A:35:GLY:C	2.61	0.44
1:A:133:ILE:HD11	1:A:191:LEU:CD1	2.46	0.44
1:B:217:ARG:HA	1:B:283:LEU:O	2.18	0.44
1:C:2:ILE:O	1:C:28:VAL:HA	2.17	0.44
1:F:182:VAL:HG12	1:F:211:THR:HG22	1.99	0.44
1:F:209:VAL:O	1:F:212:ARG:NH1	2.48	0.44
1:G:98:LEU:O	1:G:267:LEU:HG	2.18	0.44
1:I:83:ARG:O	1:I:83:ARG:HG3	2.16	0.44
1:A:98:LEU:C	1:A:267:LEU:HG	2.43	0.44
1:B:219:ARG:HD3	1:B:284:GLU:O	2.18	0.44
1:B:239:LYS:HE2	1:B:243:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:VAL:HG23	1:C:17:ALA:N	2.33	0.44
1:D:53:VAL:HG11	1:D:245:PHE:HD2	1.83	0.44
1:D:234:LYS:O	1:D:239:LYS:HE3	2.18	0.44
1:H:189:ALA:N	3:H:1274:HOH:O	2.50	0.44
1:I:101:ARG:CG	1:I:195:TYR:HE1	2.31	0.44
1:I:133:ILE:HG23	1:I:133:ILE:O	2.18	0.44
1:I:159:LEU:O	1:I:160:LYS:C	2.58	0.44
1:I:245:PHE:O	1:I:248:PHE:HB3	2.18	0.44
1:A:134:GLY:HA2	1:A:170:LYS:O	2.18	0.43
1:D:147:VAL:CG1	1:D:151:LYS:HE3	2.48	0.43
1:E:58:GLN:HA	1:E:58:GLN:OE1	2.17	0.43
1:F:103:ARG:NH2	3:F:313:HOH:O	2.34	0.43
1:H:20:PHE:HE1	1:H:244:LYS:HG2	1.83	0.43
1:H:54:PHE:HE2	1:H:62:LEU:HD23	1.83	0.43
1:I:10:LYS:HE3	1:I:32:SER:CB	2.48	0.43
1:I:80:ASN:HB3	1:I:83:ARG:HH21	1.80	0.43
1:I:103:ARG:HH21	1:I:192:ILE:HA	1.82	0.43
1:I:195:TYR:CE2	1:I:196:TYR:CE1	3.06	0.43
1:B:5:TYR:CZ	1:B:31:ASN:ND2	2.87	0.43
1:G:87:VAL:HA	1:G:88:PRO:HD3	1.82	0.43
1:H:137:PRO:HA	1:H:142:PHE:CD2	2.53	0.43
1:H:273:SER:N	3:H:1390:HOH:O	2.50	0.43
1:I:173:ALA:C	1:I:174:LYS:HG2	2.42	0.43
1:A:110:ARG:HH21	1:A:210:HIS:CD2	2.36	0.43
1:C:114:GLU:O	1:C:115:LYS:HG3	2.18	0.43
1:I:110:ARG:HH11	1:I:210:HIS:CD2	2.36	0.43
1:G:59:ILE:N	1:G:60:PRO:CD	2.82	0.43
1:H:54:PHE:CE2	1:H:62:LEU:HD23	2.52	0.43
1:I:84:GLY:N	3:I:1374:HOH:O	2.51	0.43
1:A:252:LYS:HE2	1:A:256:ARG:HH22	1.82	0.43
1:B:82:THR:HG21	1:B:97:ALA:O	2.18	0.43
1:C:3:THR:C	3:C:351:HOH:O	2.61	0.43
1:F:219:ARG:NH1	1:F:285:ALA:O	2.43	0.43
1:G:26:ILE:H	1:G:26:ILE:HG13	1.54	0.43
1:D:36:ASP:N	3:D:757:HOH:O	2.52	0.43
1:E:33:ALA:HB3	1:E:38:LEU:HD21	2.00	0.43
1:F:191:LEU:HD22	1:F:191:LEU:H	1.80	0.43
1:F:216:VAL:O	1:F:218:HIS:HD2	2.02	0.43
1:G:17:ALA:O	1:G:20:PHE:HB3	2.18	0.43
1:G:202:ARG:NH2	1:G:275:PHE:CD1	2.87	0.43
1:A:143:LEU:HA	1:A:146:ILE:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LYS:HB3	1:C:85:LYS:NZ	2.34	0.43
1:F:33:ALA:HB3	1:F:38:LEU:CD1	2.48	0.43
1:F:175:ASN:OD1	1:F:196:TYR:CE1	2.72	0.43
1:H:20:PHE:CE2	1:H:26:ILE:HB	2.54	0.43
1:H:246:VAL:HA	1:H:249:LEU:HB3	1.99	0.43
1:I:34:LYS:HD2	1:I:36:ASP:OD1	2.19	0.43
1:B:71:LEU:HB2	1:B:94:ASP:HB2	2.00	0.43
1:D:269:PRO:HD2	1:D:270:HIS:CD2	2.54	0.43
1:E:92:LYS:HB2	1:E:94:ASP:OD1	2.19	0.43
1:F:85:LYS:HE2	1:F:219:ARG:NH2	2.22	0.43
1:F:265:TYR:CB	1:F:280:ILE:CG1	2.87	0.43
1:H:98:LEU:O	1:H:267:LEU:HB2	2.16	0.43
1:B:119:LYS:HG2	3:B:669:HOH:O	2.18	0.43
1:B:239:LYS:HB3	1:B:239:LYS:HZ3	1.81	0.43
1:B:282:LYS:HA	1:B:282:LYS:HD3	1.78	0.43
1:C:48:ARG:HE	1:C:237:GLN:NE2	2.15	0.43
1:I:160:LYS:HD3	3:I:1383:HOH:O	2.19	0.43
1:I:174:LYS:HB2	3:I:365:HOH:O	2.18	0.43
1:C:162:LEU:HB3	1:C:308:MET:HE2	2.01	0.43
1:C:181:ALA:O	1:C:186:GLU:HB2	2.18	0.43
1:D:126:THR:HB	1:D:127:PRO:HD2	2.00	0.43
1:H:10:LYS:O	1:H:14:GLN:HG3	2.19	0.43
1:A:114:GLU:HA	1:A:117:LEU:HD13	2.01	0.42
1:C:82:THR:O	1:C:83:ARG:C	2.60	0.42
1:D:146:ILE:O	1:D:150:VAL:HG23	2.19	0.42
1:E:100:GLY:HA2	1:E:226:THR:O	2.19	0.42
1:F:8:GLN:CD	1:F:9:HIS:H	2.26	0.42
1:G:163:LYS:CD	1:G:306:ALA:HA	2.49	0.42
1:A:217:ARG:HA	1:A:283:LEU:O	2.19	0.42
1:A:255:GLN:HB2	1:A:271:VAL:HG21	2.01	0.42
1:C:265:TYR:CZ	1:C:283:LEU:HD11	2.54	0.42
1:D:216:VAL:HG13	3:D:314:HOH:O	2.18	0.42
1:F:36:ASP:CG	1:F:58:GLN:OE1	2.62	0.42
1:G:53:VAL:CG2	1:G:242:ALA:HB1	2.49	0.42
1:G:54:PHE:CE1	1:G:56:SER:HB2	2.54	0.42
1:H:56:SER:HB2	1:H:62:LEU:HD21	2.01	0.42
1:H:80:ASN:HA	1:H:80:ASN:HD22	1.62	0.42
1:H:135:TYR:HE2	1:H:308:MET:HE3	1.83	0.42
1:H:137:PRO:HB3	1:H:308:MET:CE	2.48	0.42
1:H:254:GLY:O	1:H:257:ALA:HB3	2.18	0.42
1:A:106:VAL:HG23	1:A:192:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:NH2	3:A:1141:HOH:O	2.52	0.42
1:B:38:LEU:HB2	1:B:54:PHE:HE1	1.84	0.42
1:G:20:PHE:CE1	1:G:244:LYS:HG2	2.50	0.42
1:G:54:PHE:O	1:G:230:ALA:HA	2.19	0.42
1:G:99:SER:HA	1:G:267:LEU:HG	2.01	0.42
1:G:137:PRO:C	1:G:138:THR:HG23	2.43	0.42
1:H:90:ALA:HA	1:H:95:TRP:CH2	2.53	0.42
1:A:166:LYS:HD3	1:A:307:GLY:O	2.19	0.42
1:C:20:PHE:CE2	1:C:26:ILE:HB	2.54	0.42
1:C:112:LEU:HD11	1:C:188:ASP:HB3	2.02	0.42
1:F:94:ASP:OD1	1:F:94:ASP:N	2.52	0.42
1:A:54:PHE:CD2	1:A:65:LEU:HD12	2.55	0.42
1:B:252:LYS:NZ	1:B:270:HIS:HB3	2.34	0.42
1:E:245:PHE:O	1:E:249:LEU:HG	2.19	0.42
1:F:95:TRP:HB3	1:F:231:ALA:HB2	2.01	0.42
1:G:72:GLU:OE1	1:G:239:LYS:NZ	2.43	0.42
1:G:252:LYS:H	1:G:252:LYS:CD	2.30	0.42
1:H:162:LEU:HD13	1:H:303:LEU:HA	2.02	0.42
1:H:273:SER:CA	3:H:1390:HOH:O	2.65	0.42
1:I:186:GLU:HB3	3:I:1382:HOH:O	2.19	0.42
1:A:7:GLY:O	1:A:57:GLU:HB2	2.19	0.42
1:B:33:ALA:O	1:B:34:LYS:C	2.61	0.42
1:C:303:LEU:HD12	1:C:303:LEU:HA	1.93	0.42
1:E:112:LEU:CD1	1:E:116:ASP:HB2	2.49	0.42
1:F:62:LEU:HD13	1:F:95:TRP:HB2	2.01	0.42
1:G:182:VAL:HA	1:G:187:ILE:O	2.20	0.42
1:E:107:TYR:CD1	1:E:117:LEU:HD11	2.55	0.42
1:F:59:ILE:N	1:F:60:PRO:CD	2.82	0.42
1:H:27:LYS:C	1:H:28:VAL:HG13	2.45	0.42
1:I:132:ARG:NE	1:I:188:ASP:OD2	2.47	0.42
1:I:153:LYS:HA	1:I:153:LYS:HD3	1.80	0.42
1:C:162:LEU:HB3	1:C:308:MET:CE	2.50	0.42
1:C:248:PHE:CE2	1:C:254:GLY:CA	3.03	0.42
1:C:256:ARG:HA	1:C:259:THR:CG2	2.50	0.42
1:E:233:LEU:HD23	1:E:233:LEU:N	2.34	0.42
1:F:147:VAL:CG2	1:F:295:GLU:HG3	2.41	0.42
1:G:233:LEU:N	1:G:233:LEU:CD1	2.82	0.42
1:G:265:TYR:HA	1:G:266:PRO:HD3	1.91	0.42
1:H:265:TYR:CE2	1:H:283:LEU:HD11	2.54	0.42
1:D:144:GLU:HG2	1:D:224:LEU:HD21	2.02	0.42
1:D:234:LYS:C	1:D:236:SER:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:ASN:CB	1:F:196:TYR:CE1	3.02	0.42
1:G:146:ILE:CG1	1:G:162:LEU:HD21	2.49	0.42
1:G:175:ASN:HD22	1:G:192:ILE:HG22	1.85	0.42
1:I:5:TYR:CZ	1:I:51:ALA:HB2	2.55	0.42
1:I:43:LYS:HD2	1:I:43:LYS:O	2.19	0.42
1:I:268:ASN:HA	1:I:269:PRO:HD3	1.87	0.42
1:B:67:ALA:C	1:B:69:ASN:N	2.78	0.42
1:F:300:THR:O	1:F:303:LEU:HB2	2.19	0.42
1:I:195:TYR:HE2	1:I:196:TYR:CZ	2.38	0.42
1:C:30:LEU:HA	1:C:30:LEU:HD23	1.77	0.41
1:E:1:ASP:OD1	1:E:27:LYS:HB2	2.20	0.41
1:F:273:SER:OG	3:F:1091:HOH:O	2.22	0.41
1:A:59:ILE:N	1:A:60:PRO:HD2	2.35	0.41
1:A:142:PHE:HE2	1:A:303:LEU:HD21	1.86	0.41
1:B:119:LYS:O	1:B:216:VAL:HG13	2.20	0.41
1:C:220:ASP:CG	1:C:221:PRO:HD2	2.45	0.41
1:C:283:LEU:HD23	1:C:283:LEU:HA	1.83	0.41
1:D:146:ILE:HD11	1:D:303:LEU:HD21	2.01	0.41
1:D:217:ARG:HH11	1:D:217:ARG:CG	2.33	0.41
1:D:265:TYR:HB3	1:D:280:ILE:HG12	2.01	0.41
1:E:112:LEU:CD1	1:E:116:ASP:CB	2.98	0.41
3:A:1457:HOH:O	1:H:237:GLN:NE2	2.54	0.41
1:D:113:SER:HB3	1:D:115:LYS:HD3	2.01	0.41
1:D:220:ASP:OD1	1:D:221:PRO:HD2	2.20	0.41
1:H:39:ALA:C	1:H:41:GLN:H	2.28	0.41
1:H:59:ILE:N	1:H:60:PRO:CD	2.83	0.41
1:I:174:LYS:HB3	1:I:174:LYS:HE2	1.83	0.41
1:A:5:TYR:CE1	1:A:51:ALA:HB2	2.55	0.41
1:B:152:LEU:HD11	1:B:286:PRO:HB2	2.02	0.41
1:B:268:ASN:OD1	1:B:269:PRO:HD2	2.21	0.41
1:C:8:GLN:O	1:C:9:HIS:C	2.62	0.41
1:C:159:LEU:CG	1:C:163:LYS:HE3	2.50	0.41
1:D:9:HIS:NE2	1:D:11:GLU:OE2	2.54	0.41
1:D:266:PRO:O	1:D:280:ILE:HD11	2.21	0.41
1:D:301:ARG:HA	1:D:301:ARG:HD2	1.83	0.41
1:E:287:GLN:H	1:E:287:GLN:HG2	1.73	0.41
1:F:12:ALA:O	1:F:16:VAL:HG23	2.19	0.41
1:G:265:TYR:HB2	1:G:280:ILE:HD11	2.01	0.41
1:G:267:LEU:HD23	1:G:280:ILE:HD12	2.02	0.41
1:I:55:TYR:HE1	1:I:98:LEU:HD12	1.86	0.41
1:I:96:VAL:HG22	1:I:97:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:GLU:HG2	1:I:129:TRP:CZ2	2.55	0.41
1:A:300:THR:CG2	1:A:309:LYS:HE3	2.50	0.41
1:F:256:ARG:HG2	1:F:271:VAL:HG13	2.01	0.41
1:G:80:ASN:OD1	1:G:83:ARG:NH2	2.42	0.41
1:G:101:ARG:HG2	1:G:195:TYR:CD1	2.56	0.41
1:H:66:SER:OG	1:H:92:LYS:HB2	2.20	0.41
1:H:265:TYR:CZ	1:H:283:LEU:HD11	2.55	0.41
1:I:292:THR:HG23	3:I:763:HOH:O	2.20	0.41
1:A:72:GLU:OE1	1:A:239:LYS:HE2	2.20	0.41
1:B:4:VAL:O	1:B:31:ASN:N	2.53	0.41
1:B:240:ASP:O	1:B:244:LYS:HG3	2.20	0.41
1:B:243:LYS:HB3	3:B:1385:HOH:O	2.20	0.41
1:E:136:VAL:HA	1:E:137:PRO:HD2	1.89	0.41
1:F:5:TYR:CD1	1:F:51:ALA:HB2	2.56	0.41
1:F:133:ILE:HD11	1:F:191:LEU:CD2	2.50	0.41
1:I:81:GLU:CD	1:I:251:GLY:HA2	2.45	0.41
1:D:170:LYS:HA	1:D:171:PRO:HD3	1.93	0.41
1:E:265:TYR:N	1:E:265:TYR:CD1	2.89	0.41
1:F:170:LYS:HE2	3:F:1488:HOH:O	2.21	0.41
1:G:62:LEU:HD13	1:G:95:TRP:HB2	2.02	0.41
1:H:3:THR:N	3:H:1069:HOH:O	2.52	0.41
1:H:216:VAL:O	1:H:217:ARG:HB2	2.21	0.41
1:I:96:VAL:O	1:I:229:GLY:HA2	2.21	0.41
1:D:104:VAL:CG2	1:D:105:VAL:N	2.83	0.41
1:E:89:VAL:HG13	3:E:1259:HOH:O	2.20	0.41
1:E:162:LEU:O	1:E:308:MET:HE3	2.21	0.41
1:F:220:ASP:O	1:F:286:PRO:HG3	2.21	0.41
1:I:195:TYR:HA	1:I:263:ALA:HB3	2.01	0.41
1:A:65:LEU:O	1:A:71:LEU:HG	2.21	0.41
1:B:198:HIS:CE1	3:B:1444:HOH:O	2.73	0.41
1:C:79:ILE:CD1	1:C:93:LYS:HG3	2.49	0.41
1:C:193:ASN:HB3	1:C:195:TYR:CE1	2.56	0.41
1:D:6:ASN:O	1:D:32:SER:HA	2.21	0.41
1:D:16:VAL:HG13	1:D:248:PHE:HE2	1.85	0.41
1:E:66:SER:OG	1:E:92:LYS:HD3	2.21	0.41
1:E:256:ARG:HA	1:E:259:THR:HG22	2.02	0.41
1:G:304:GLU:O	1:G:305:GLN:C	2.63	0.41
1:H:97:ALA:HA	1:H:228:SER:O	2.21	0.41
1:I:54:PHE:CE2	1:I:56:SER:HB2	2.55	0.41
1:D:53:VAL:HG12	1:D:242:ALA:HB1	2.03	0.41
1:D:94:ASP:OD1	1:D:94:ASP:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ALA:HB2	3:D:324:HOH:O	2.20	0.41
1:F:85:LYS:HZ2	1:F:219:ARG:NH1	2.19	0.41
1:H:75:PRO:C	1:H:77:SER:H	2.29	0.41
1:I:129:TRP:O	1:I:130:LYS:O	2.37	0.41
1:I:265:TYR:CE2	1:I:283:LEU:HD11	2.56	0.41
1:A:66:SER:HB2	1:A:71:LEU:HD12	2.03	0.40
1:B:134:GLY:HA2	1:B:170:LYS:O	2.21	0.40
1:D:149:ILE:HG13	1:D:221:PRO:HB3	2.03	0.40
1:D:161:TRP:CZ2	1:D:165:LEU:HD11	2.56	0.40
1:D:198:HIS:NE2	3:D:1446:HOH:O	2.37	0.40
1:G:265:TYR:CB	1:G:280:ILE:HD11	2.51	0.40
1:H:54:PHE:O	1:H:231:ALA:N	2.53	0.40
1:B:98:LEU:HG	1:B:229:GLY:HA2	2.04	0.40
1:B:130:LYS:HE3	1:B:131:ASN:ND2	2.36	0.40
1:B:253:GLU:H	1:B:253:GLU:HG3	1.51	0.40
1:B:292:THR:OG1	1:B:295:GLU:HB2	2.21	0.40
1:D:78:THR:HG23	1:D:247:ALA:HA	2.03	0.40
1:E:57:GLU:O	1:E:101:ARG:NH2	2.54	0.40
1:E:259:THR:O	1:E:274:THR:HG22	2.22	0.40
1:F:182:VAL:O	1:F:184:ASN:N	2.55	0.40
1:G:244:LYS:NZ	3:G:712:HOH:O	2.54	0.40
1:G:265:TYR:CD1	1:G:265:TYR:N	2.89	0.40
1:H:189:ALA:C	3:H:1274:HOH:O	2.65	0.40
1:B:59:ILE:N	1:B:60:PRO:CD	2.84	0.40
1:C:155:GLU:O	1:C:158:ALA:HB3	2.21	0.40
1:D:104:VAL:HG21	1:D:213:LEU:HB3	2.04	0.40
1:D:210:HIS:CE1	3:D:795:HOH:O	2.73	0.40
1:G:2:ILE:HA	1:G:52:ASP:OD1	2.21	0.40
1:H:42:ILE:HG21	1:H:233:LEU:CD1	2.52	0.40
1:I:183:GLU:OE2	1:I:211:THR:HG23	2.21	0.40
1:I:248:PHE:HA	3:I:873:HOH:O	2.20	0.40
3:A:1179:HOH:O	1:H:48:ARG:HG2	2.20	0.40
1:B:256:ARG:HD3	3:B:796:HOH:O	2.21	0.40
1:C:111:LYS:HE2	1:C:111:LYS:HB3	1.54	0.40
1:D:260:ALA:HA	1:D:274:THR:CG2	2.52	0.40
1:F:170:LYS:HA	1:F:171:PRO:HD3	1.93	0.40
1:H:292:THR:H	1:H:295:GLU:HB2	1.86	0.40
1:I:173:ALA:O	1:I:174:LYS:HG2	2.22	0.40
1:A:115:LYS:NZ	1:A:115:LYS:CB	2.77	0.40
1:A:170:LYS:HE3	1:A:170:LYS:HB2	1.93	0.40
1:B:170:LYS:CE	1:B:187:ILE:HD12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:TYR:O	1:C:211:THR:HA	2.22	0.40
1:C:204:LYS:CE	3:C:1506:HOH:O	2.61	0.40
1:I:107:TYR:CD1	1:I:117:LEU:HD11	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/309 (99%)	297 (97%)	10 (3%)	0	100	100
1	B	307/309 (99%)	280 (91%)	21 (7%)	6 (2%)	6	2
1	C	307/309 (99%)	284 (92%)	18 (6%)	5 (2%)	7	4
1	D	307/309 (99%)	286 (93%)	16 (5%)	5 (2%)	7	4
1	E	307/309 (99%)	296 (96%)	9 (3%)	2 (1%)	18	15
1	F	307/309 (99%)	284 (92%)	18 (6%)	5 (2%)	7	4
1	G	307/309 (99%)	284 (92%)	19 (6%)	4 (1%)	9	6
1	H	307/309 (99%)	262 (85%)	39 (13%)	6 (2%)	6	2
1	I	307/309 (99%)	274 (89%)	30 (10%)	3 (1%)	12	9
All	All	2763/2781 (99%)	2547 (92%)	180 (6%)	36 (1%)	9	6

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	85	LYS
1	H	8	GLN
1	H	81	GLU
1	B	33	ALA
1	B	85	LYS

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Mol	Chain	Res	Type
1	C	85	LYS
1	C	114	GLU
1	D	240	ASP
1	E	44	GLU
1	F	183	GLU
1	F	185	GLY
1	G	26	ILE
1	H	12	ALA
1	C	46	GLY
1	C	47	SER
1	C	279	PRO
1	D	217	ARG
1	D	239	LYS
1	F	116	ASP
1	H	11	GLU
1	I	130	LYS
1	I	307	GLY
1	D	155	GLU
1	E	45	GLU
1	F	33	ALA
1	G	23	ALA
1	G	217	ARG
1	H	10	LYS
1	H	69	ASN
1	I	203	GLU
1	B	93	LYS
1	D	156	ALA
1	B	240	ASP
1	B	276	ASN
1	G	192	ILE
1	B	73	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/245 (100%)	227 (93%)	18 (7%)	13	10
1	B	245/245 (100%)	225 (92%)	20 (8%)	10	8
1	C	245/245 (100%)	225 (92%)	20 (8%)	10	8
1	D	245/245 (100%)	222 (91%)	23 (9%)	8	6
1	E	245/245 (100%)	225 (92%)	20 (8%)	10	8
1	F	245/245 (100%)	232 (95%)	13 (5%)	20	19
1	G	245/245 (100%)	224 (91%)	21 (9%)	10	7
1	H	245/245 (100%)	216 (88%)	29 (12%)	5	3
1	I	245/245 (100%)	211 (86%)	34 (14%)	3	2
All	All	2205/2205 (100%)	2007 (91%)	198 (9%)	9	6

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	16	VAL
1	A	29	LYS
1	A	45	GLU
1	A	77	SER
1	A	92	LYS
1	A	115	LYS
1	A	121	VAL
1	A	138	THR
1	A	146	ILE
1	A	187	ILE
1	A	191	LEU
1	A	203	GLU
1	A	206	VAL
1	A	209	VAL
1	A	216	VAL
1	A	272	VAL
1	A	302	LEU
1	B	3	THR
1	B	8	GLN
1	B	16	VAL
1	B	30	LEU
1	B	34	LYS

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Mol	Chain	Res	Type
1	B	44	GLU
1	B	78	THR
1	B	93	LYS
1	B	112	LEU
1	B	114	GLU
1	B	167	GLU
1	B	183	GLU
1	B	191	LEU
1	B	211	THR
1	B	218	HIS
1	B	239	LYS
1	B	240	ASP
1	B	253	GLU
1	B	259	THR
1	B	293	VAL
1	C	8	GLN
1	C	10	LYS
1	C	11	GLU
1	C	28	VAL
1	C	29	LYS
1	C	79	ILE
1	C	81	GLU
1	C	85	LYS
1	C	115	LYS
1	C	167	GLU
1	C	183	GLU
1	C	204	LYS
1	C	207	GLN
1	C	209	VAL
1	C	211	THR
1	C	253	GLU
1	C	258	LEU
1	C	268	ASN
1	C	274	THR
1	C	293	VAL
1	D	1	ASP
1	D	9	HIS
1	D	10	LYS
1	D	11	GLU
1	D	53	VAL
1	D	65	LEU
1	D	101	ARG

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Mol	Chain	Res	Type
1	D	115	LYS
1	D	204	LYS
1	D	214	ASN
1	D	235	SER
1	D	237	GLN
1	D	239	LYS
1	D	240	ASP
1	D	252	LYS
1	D	256	ARG
1	D	259	THR
1	D	264	GLU
1	D	268	ASN
1	D	280	ILE
1	D	287	GLN
1	D	308	MET
1	D	309	LYS
1	E	3	THR
1	E	29	LYS
1	E	32	SER
1	E	36	ASP
1	E	96	VAL
1	E	101	ARG
1	E	121	VAL
1	E	152	LEU
1	E	163	LYS
1	E	191	LEU
1	E	200	PHE
1	E	219	ARG
1	E	233	LEU
1	E	252	LYS
1	E	253	GLU
1	E	268	ASN
1	E	274	THR
1	E	280	ILE
1	E	301	ARG
1	E	309	LYS
1	F	8	GLN
1	F	9	HIS
1	F	38	LEU
1	F	64	THR
1	F	103	ARG
1	F	166	LYS

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Mol	Chain	Res	Type
1	F	180	GLN
1	F	184	ASN
1	F	186	GLU
1	F	191	LEU
1	F	233	LEU
1	F	280	ILE
1	F	287	GLN
1	G	8	GLN
1	G	18	ASP
1	G	38	LEU
1	G	58	GLN
1	G	74	LEU
1	G	104	VAL
1	G	112	LEU
1	G	114	GLU
1	G	146	ILE
1	G	159	LEU
1	G	163	LYS
1	G	206	VAL
1	G	233	LEU
1	G	234	LYS
1	G	240	ASP
1	G	252	LYS
1	G	264	GLU
1	G	280	ILE
1	G	297	GLU
1	G	303	LEU
1	G	304	GLU
1	H	2	ILE
1	H	3	THR
1	H	30	LEU
1	H	34	LYS
1	H	36	ASP
1	H	37	GLN
1	H	38	LEU
1	H	52	ASP
1	H	69	ASN
1	H	70	LEU
1	H	80	ASN
1	H	89	VAL
1	H	92	LYS
1	H	93	LYS

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Mol	Chain	Res	Type
1	H	99	SER
1	H	117	LEU
1	H	135	TYR
1	H	153	LYS
1	H	155	GLU
1	H	206	VAL
1	H	218	HIS
1	H	233	LEU
1	H	249	LEU
1	H	253	GLU
1	H	255	GLN
1	H	264	GLU
1	H	288	VAL
1	H	295	GLU
1	H	297	GLU
1	I	8	GLN
1	I	16	VAL
1	I	22	ARG
1	I	24	THR
1	I	29	LYS
1	I	30	LEU
1	I	43	LYS
1	I	62	LEU
1	I	66	SER
1	I	70	LEU
1	I	71	LEU
1	I	72	GLU
1	I	80	ASN
1	I	83	ARG
1	I	85	LYS
1	I	109	THR
1	I	111	LYS
1	I	122	LEU
1	I	167	GLU
1	I	177	VAL
1	I	204	LYS
1	I	212	ARG
1	I	213	LEU
1	I	226	THR
1	I	234	LYS
1	I	239	LYS
1	I	240	ASP

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Mol	Chain	Res	Type
1	I	253	GLU
1	I	267	LEU
1	I	274	THR
1	I	277	LEU
1	I	288	VAL
1	I	296	LYS
1	I	300	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	9	HIS
1	A	198	HIS
1	A	208	ASN
1	A	210	HIS
1	A	218	HIS
1	A	255	GLN
1	A	298	HIS
1	B	9	HIS
1	B	41	GLN
1	B	131	ASN
1	B	175	ASN
1	B	193	ASN
1	B	198	HIS
1	B	210	HIS
1	B	214	ASN
1	B	238	ASN
1	B	298	HIS
1	C	8	GLN
1	C	31	ASN
1	C	175	ASN
1	C	180	GLN
1	C	198	HIS
1	C	208	ASN
1	C	237	GLN
1	C	255	GLN
1	C	268	ASN
1	C	270	HIS
1	D	14	GLN
1	D	37	GLN
1	D	123	ASN

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Mol	Chain	Res	Type
1	D	175	ASN
1	D	193	ASN
1	D	210	HIS
1	D	238	ASN
1	D	268	ASN
1	D	270	HIS
1	D	298	HIS
1	E	6	ASN
1	E	37	GLN
1	E	69	ASN
1	E	123	ASN
1	E	198	HIS
1	E	237	GLN
1	E	238	ASN
1	E	255	GLN
1	F	80	ASN
1	F	145	GLN
1	F	175	ASN
1	F	198	HIS
1	F	214	ASN
1	F	218	HIS
1	F	238	ASN
1	F	255	GLN
1	F	276	ASN
1	F	287	GLN
1	F	298	HIS
1	G	69	ASN
1	G	175	ASN
1	G	184	ASN
1	G	237	GLN
1	G	255	GLN
1	H	37	GLN
1	H	69	ASN
1	H	80	ASN
1	H	131	ASN
1	H	175	ASN
1	H	180	GLN
1	H	184	ASN
1	H	208	ASN
1	H	255	GLN
1	I	6	ASN
1	I	8	GLN

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Mol	Chain	Res	Type
1	I	31	ASN
1	I	69	ASN
1	I	80	ASN
1	I	175	ASN
1	I	214	ASN
1	I	238	ASN
1	I	270	HIS
1	I	298	HIS
1	I	305	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	309/309 (100%)	-0.79	0 100 100	12, 20, 31, 41	0
1	B	309/309 (100%)	-0.50	0 100 100	11, 23, 45, 62	0
1	C	309/309 (100%)	-0.67	0 100 100	12, 23, 37, 55	0
1	D	309/309 (100%)	-0.57	0 100 100	15, 26, 38, 51	0
1	E	309/309 (100%)	-0.76	0 100 100	13, 23, 34, 46	0
1	F	309/309 (100%)	-0.69	1 (0%) 90 91	13, 22, 36, 48	0
1	G	309/309 (100%)	-0.48	0 100 100	18, 29, 41, 50	0
1	H	309/309 (100%)	0.03	3 (0%) 79 81	23, 38, 59, 65	0
1	I	309/309 (100%)	-0.19	1 (0%) 90 91	22, 36, 49, 67	0
All	All	2781/2781 (100%)	-0.51	5 (0%) 91 92	11, 27, 48, 67	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	242	ALA	3.3
1	H	16	VAL	2.9
1	H	30	LEU	2.5
1	I	308	MET	2.2
1	F	85	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CU	F	310	1/1	0.89	0.08	53,53,53,53	0
2	CU	F	311	1/1	0.93	0.06	61,61,61,61	0
2	CU	H	311	1/1	0.93	0.07	71,71,71,71	0
2	CU	G	311	1/1	0.97	0.05	55,55,55,55	0
2	CU	I	311	1/1	0.97	0.05	64,64,64,64	0
2	CU	G	310	1/1	0.98	0.04	53,53,53,53	0
2	CU	D	311	1/1	0.98	0.04	50,50,50,50	0
2	CU	H	310	1/1	0.98	0.04	56,56,56,56	0
2	CU	B	311	1/1	0.98	0.03	46,46,46,46	0
2	CU	C	310	1/1	0.98	0.03	49,49,49,49	0
2	CU	A	310	1/1	0.99	0.02	38,38,38,38	0
2	CU	E	310	1/1	0.99	0.03	46,46,46,46	0
2	CU	E	311	1/1	0.99	0.03	45,45,45,45	0
2	CU	B	310	1/1	0.99	0.03	41,41,41,41	0
2	CU	D	310	1/1	0.99	0.05	45,45,45,45	0
2	CU	C	311	1/1	1.00	0.02	37,37,37,37	0
2	CU	I	310	1/1	1.00	0.02	46,46,46,46	0
2	CU	A	311	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.