



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:51 PM EDT

PDB ID : 1M5H / pdb_00001m5h
Title : Formylmethanofuran:tetrahydromethanopterin formyltransferase from
Archaeoglobus fulgidus
Authors : Mamat, B.; Roth, A.; Grimm, C.; Ermler, U.; Tziatzios, C.; Schubert, D.;
Thauer, R.K.; Shima, S.
Deposited on : 2002-07-09
Resolution : 2.00 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:

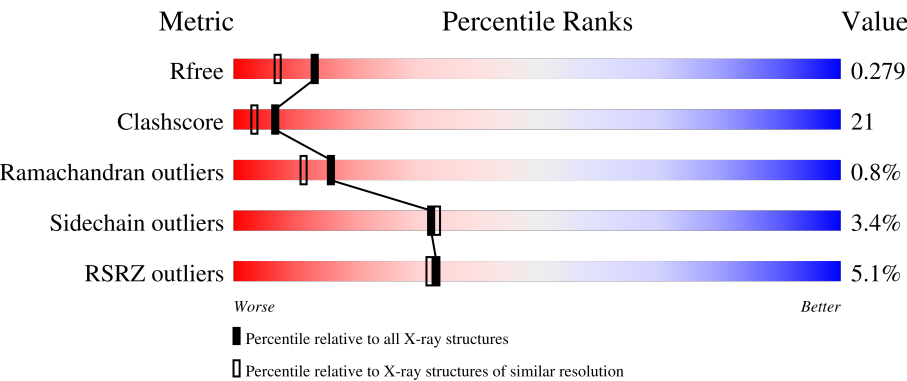
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	297	3% 66% 31% .
1	B	297	5% 63% 33% .
1	C	297	3% 66% 31% .
1	D	297	8% 64% 33% .
1	E	297	8% 63% 34% .

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Mol	Chain	Length	Quality of chain
1	F	297	3% 66% 32%
1	G	297	4% 64% 32%
1	H	297	5% 64% 34%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19658 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 Formylmethanofuran--tetrahydromethanopterin formyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2230	1429	365	426	10			
1	B	297	Total	C	N	O	S	0	0	0
			2230	1429	365	426	10			
1	C	297	Total	C	N	O	S	0	0	0
			2230	1429	365	426	10			
1	D	297	Total	C	N	O	S	0	0	0
			2230	1429	365	426	10			
1	E	297	Total	C	N	O	S	0	0	0
			2230	1429	365	426	10			
1	F	297	Total	C	N	O	S	0	0	0
			2230	1429	365	426	10			
1	G	297	Total	C	N	O	S	0	0	0
			2230	1429	365	426	10			
1	H	297	Total	C	N	O	S	0	0	0
			2230	1429	365	426	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	ASP	PHE	conflict	UNP O28076
A	129	GLN	GLU	conflict	UNP O28076
A	239	ALA	GLU	conflict	UNP O28076
B	1115	ASP	PHE	conflict	UNP O28076
B	1129	GLN	GLU	conflict	UNP O28076
B	1239	ALA	GLU	conflict	UNP O28076
C	2115	ASP	PHE	conflict	UNP O28076
C	2129	GLN	GLU	conflict	UNP O28076
C	2239	ALA	GLU	conflict	UNP O28076
D	3115	ASP	PHE	conflict	UNP O28076
D	3129	GLN	GLU	conflict	UNP O28076
D	3239	ALA	GLU	conflict	UNP O28076

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Chain	Residue	Modelled	Actual	Comment	Reference
E	4115	ASP	PHE	conflict	UNP O28076
E	4129	GLN	GLU	conflict	UNP O28076
E	4239	ALA	GLU	conflict	UNP O28076
F	5115	ASP	PHE	conflict	UNP O28076
F	5129	GLN	GLU	conflict	UNP O28076
F	5239	ALA	GLU	conflict	UNP O28076
G	6115	ASP	PHE	conflict	UNP O28076
G	6129	GLN	GLU	conflict	UNP O28076
G	6239	ALA	GLU	conflict	UNP O28076
H	7115	ASP	PHE	conflict	UNP O28076
H	7129	GLN	GLU	conflict	UNP O28076
H	7239	ALA	GLU	conflict	UNP O28076

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	231	Total O 231 231	0	0
3	B	225	Total O 225 225	0	0
3	C	226	Total O 226 226	0	0

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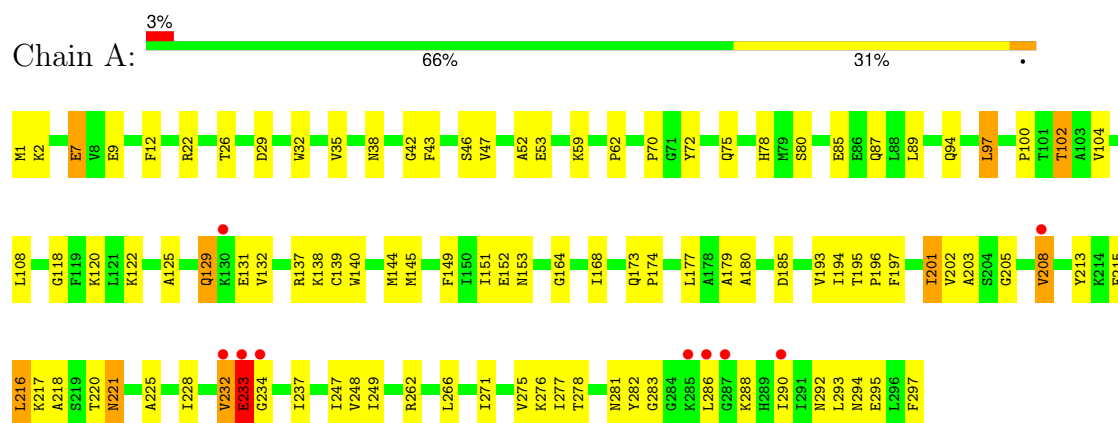
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	215	Total 215	O 215	0	0
3	E	239	Total 239	O 239	0	0
3	F	226	Total 226	O 226	0	0
3	G	206	Total 206	O 206	0	0
3	H	226	Total 226	O 226	0	0

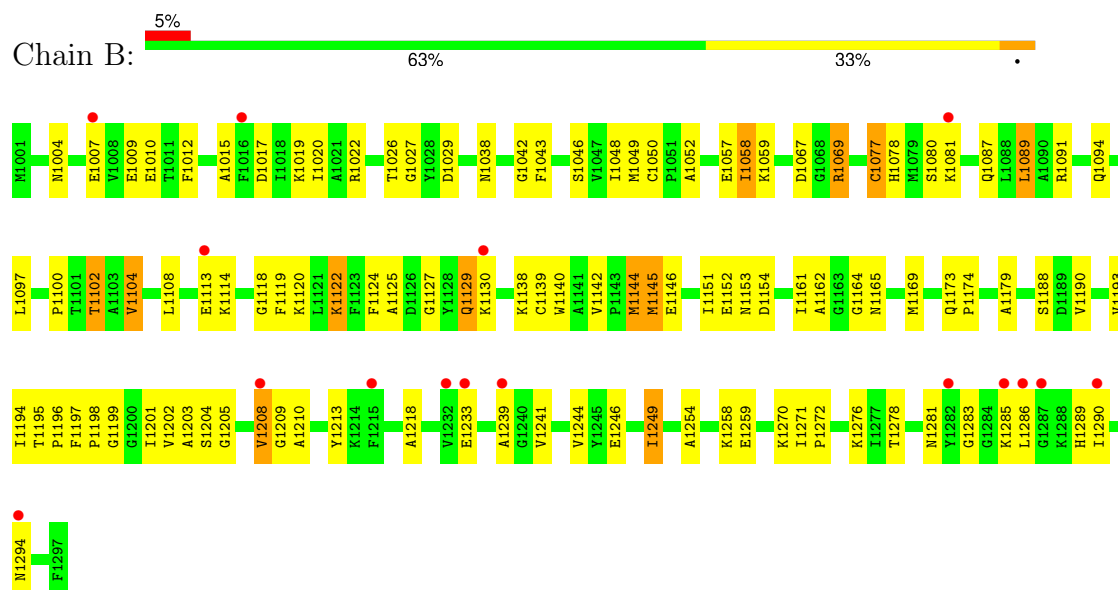
3 Residue-property plots [i](#)

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: Formylmethanofuran--tetrahydromethanopterin formyltransferase

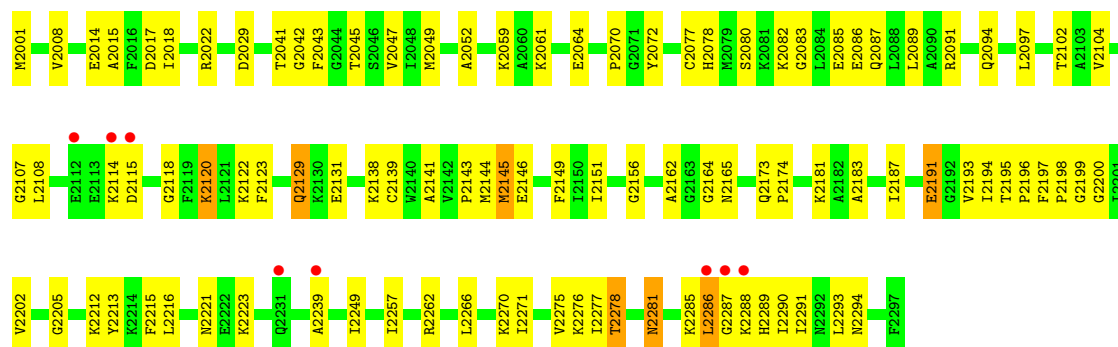


- Molecule 1: Formylmethanofuran--tetrahydromethanopterin formyltransferase

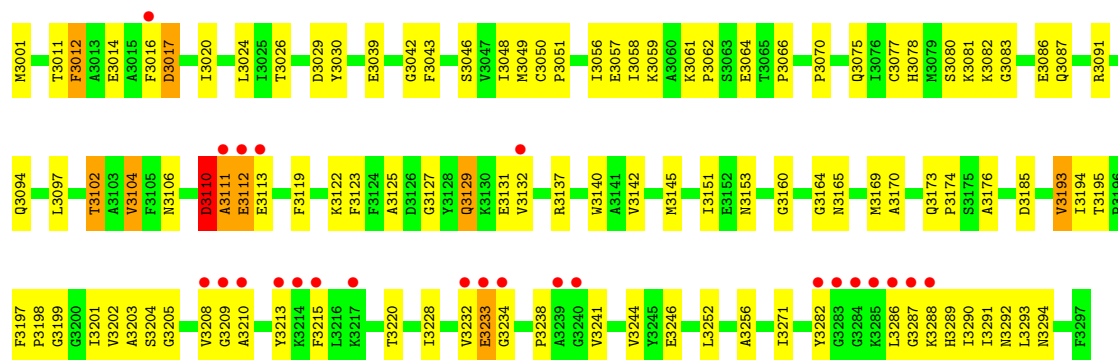


- Molecule 1: Formylmethanofuran--tetrahydromethanopterin formyltransferase

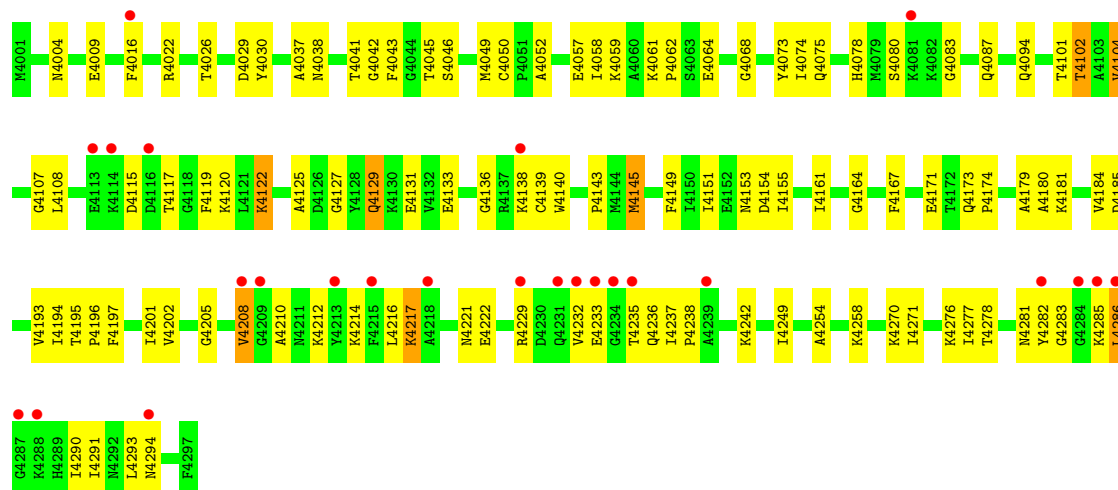




• Molecule 1: Formylmethanofuran--tetrahydromethanopterin formyltransferase

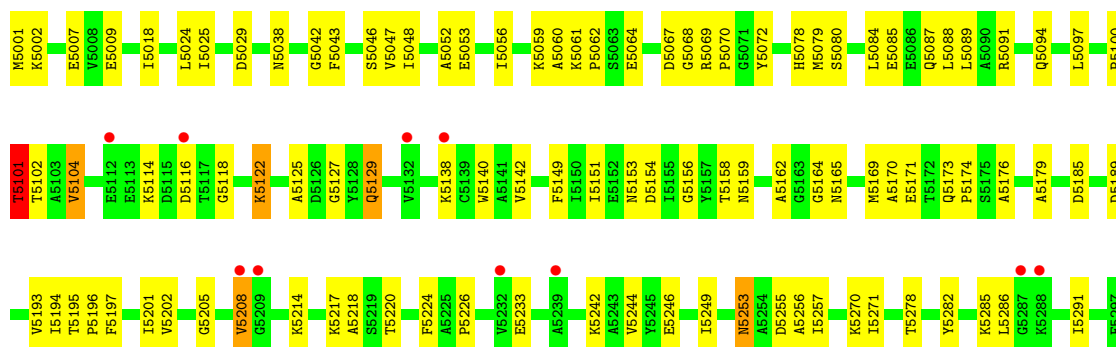


• Molecule 1: Formylmethanofuran--tetrahydromethanopterin formyltransferase

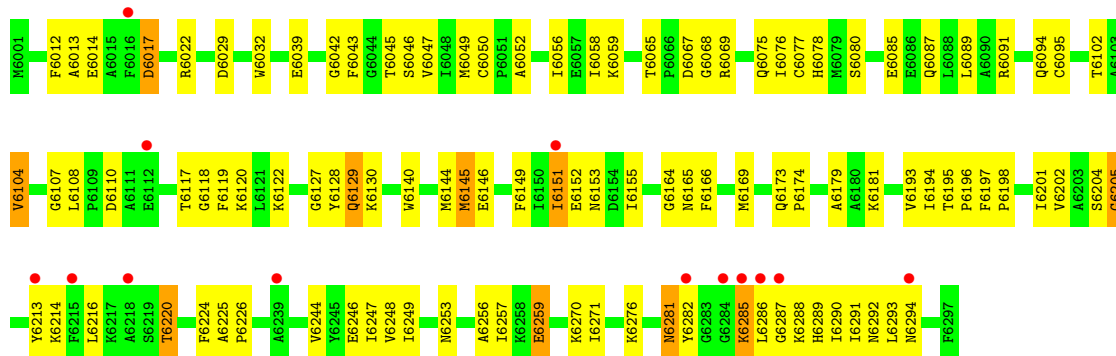


• Molecule 1: Formylmethanofuran--tetrahydromethanopterin formyltransferase

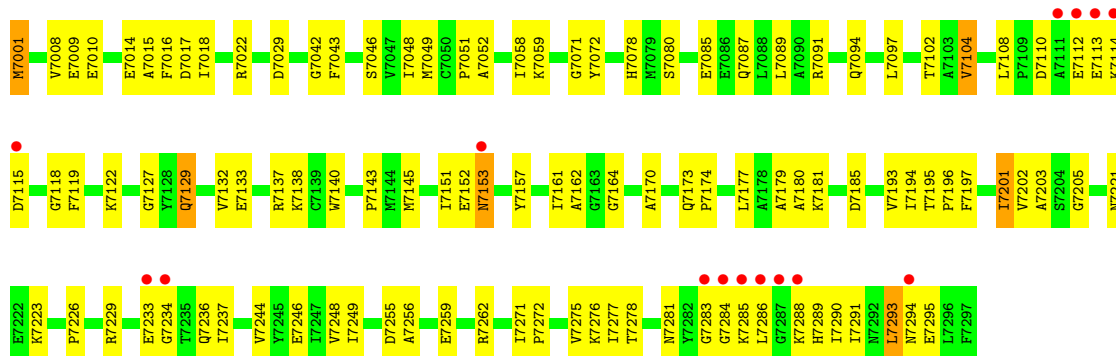




• Molecule 1: Formylmethanofuran--tetrahydromethanopterin formyltransferase



• Molecule 1: Formylmethanofuran--tetrahydromethanopterin formyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.10Å 81.81Å 99.10Å 90.10° 110.04° 93.75°	Depositor
Resolution (Å)	29.25 – 2.00 29.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	82.2 (29.25-2.00) 82.3 (29.25-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.282 0.226 , 0.279	Depositor DCC
R_{free} test set	6699 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19658	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.90% 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:
K

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	0.44	0/2274	0.97	13/3078 (0.4%)
1	B	0.43	0/2274	0.98	14/3078 (0.5%)
1	C	0.43	0/2274	0.98	11/3078 (0.4%)
1	D	0.42	0/2274	0.96	9/3078 (0.3%)
1	E	0.42	0/2274	0.98	12/3078 (0.4%)
1	F	0.43	0/2274	0.96	10/3078 (0.3%)
1	G	0.41	0/2274	1.01	14/3078 (0.5%)
1	H	0.43	0/2274	0.97	9/3078 (0.3%)
All	All	0.43	0/18192	0.98	92/24624 (0.4%)

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	5195	THR	CA-C-N	9.36	129.11	119.56
1	F	5195	THR	C-N-CA	9.36	129.11	119.56
1	G	6164	GLY	N-CA-C	-8.77	101.84	111.93
1	E	4164	GLY	N-CA-C	-8.45	102.22	111.93
1	F	5164	GLY	N-CA-C	-8.41	102.26	111.93
1	D	3195	THR	CA-C-N	8.31	129.11	119.47
1	D	3195	THR	C-N-CA	8.31	129.11	119.47
1	B	1195	THR	CA-C-N	8.25	128.35	119.28
1	B	1195	THR	C-N-CA	8.25	128.35	119.28
1	D	3164	GLY	N-CA-C	-8.14	101.64	112.14
1	C	2195	THR	CA-C-N	8.10	127.83	119.56
1	C	2195	THR	C-N-CA	8.10	127.83	119.56
1	A	195	THR	CA-C-N	7.91	127.62	119.56
1	A	195	THR	C-N-CA	7.91	127.62	119.56
1	B	1164	GLY	N-CA-C	-7.89	102.85	111.93
1	G	6195	THR	CA-C-N	7.86	127.57	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6195	THR	C-N-CA	7.86	127.57	119.56
1	C	2271	ILE	N-CA-C	7.78	115.61	107.76
1	E	4195	THR	CA-C-N	7.58	127.30	119.56
1	E	4195	THR	C-N-CA	7.58	127.30	119.56
1	H	7195	THR	CA-C-N	7.36	126.99	119.56
1	H	7195	THR	C-N-CA	7.36	126.99	119.56
1	H	7295	GLU	N-CA-C	-7.21	104.35	113.72
1	A	164	GLY	N-CA-C	-7.13	103.73	111.93
1	H	7293	LEU	N-CA-C	7.12	118.69	111.07
1	C	2164	GLY	N-CA-C	-7.01	103.86	111.93
1	H	7164	GLY	N-CA-C	-6.81	104.09	111.93
1	F	5196	PRO	N-CA-C	6.75	122.61	113.84
1	A	196	PRO	N-CA-C	6.61	122.44	113.84
1	B	1165	ASN	N-CA-C	6.38	117.84	108.14
1	G	6145	MET	N-CA-C	6.37	118.75	111.11
1	C	2196	PRO	N-CA-C	6.31	122.04	113.84
1	G	6196	PRO	N-CA-C	6.24	121.96	113.84
1	D	3199	GLY	N-CA-C	-6.18	106.41	115.30
1	B	1102	THR	N-CA-C	6.13	118.44	110.53
1	C	2102	THR	N-CA-C	6.11	118.59	110.53
1	A	102	THR	N-CA-C	6.10	118.42	110.43
1	A	275	VAL	N-CA-C	6.04	117.01	111.81
1	B	1196	PRO	N-CA-C	6.03	121.78	113.65
1	F	5101	THR	N-CA-C	5.98	120.38	113.38
1	E	4196	PRO	N-CA-C	5.98	121.61	113.84
1	B	1233	GLU	N-CA-C	5.96	117.86	111.36
1	G	6225	ALA	CA-C-N	5.96	126.11	119.32
1	G	6225	ALA	C-N-CA	5.96	126.11	119.32
1	H	7196	PRO	N-CA-C	5.95	121.30	113.86
1	C	2139	CYS	N-CA-C	5.90	117.56	109.18
1	H	7201	ILE	N-CA-C	5.85	116.90	108.48
1	E	4102	THR	N-CA-C	5.83	118.22	110.53
1	B	1241	VAL	N-CA-C	5.83	117.14	108.23
1	B	1199	GLY	N-CA-C	-5.81	106.93	115.30
1	G	6102	THR	N-CA-C	5.80	118.19	110.53
1	D	3102	THR	N-CA-C	5.72	118.08	110.53
1	F	5165	ASN	N-CA-C	5.69	115.90	107.88
1	B	1145	MET	N-CA-C	5.68	117.93	111.11
1	G	6201	ILE	N-CA-C	5.63	116.59	108.48
1	D	3201	ILE	N-CA-C	5.60	116.55	108.48
1	B	1201	ILE	N-CA-C	5.59	116.53	108.48
1	A	100	PRO	N-CA-C	5.57	119.61	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4208	VAL	N-CA-C	5.56	116.19	110.36
1	B	1239	ALA	N-CA-C	5.54	117.76	111.11
1	H	7102	THR	N-CA-C	5.53	118.02	110.55
1	C	2165	ASN	N-CA-C	5.53	115.68	107.88
1	D	3165	ASN	N-CA-C	5.52	116.53	108.14
1	E	4201	ILE	N-CA-C	5.51	116.41	108.48
1	B	1139	CYS	N-CA-C	5.50	116.98	109.18
1	C	2275	VAL	N-CA-C	5.49	116.53	111.81
1	F	5201	ILE	N-CA-C	5.42	116.29	108.48
1	E	4139	CYS	N-CA-C	5.42	116.87	109.18
1	F	5102	THR	N-CA-C	5.42	117.52	110.53
1	A	139	CYS	N-CA-C	5.41	116.86	109.18
1	C	2199	GLY	N-CA-C	-5.40	107.53	115.30
1	E	4205	GLY	N-CA-C	-5.39	105.95	112.48
1	D	3252	LEU	N-CA-C	5.36	117.87	111.71
1	G	6165	ASN	N-CA-C	5.34	116.26	108.14
1	H	7205	GLY	N-CA-C	-5.32	105.73	112.65
1	B	1249	ILE	N-CA-C	5.32	115.64	107.77
1	G	6205	GLY	N-CA-C	-5.26	105.82	112.65
1	A	225	ALA	CA-C-N	5.25	125.30	119.32
1	A	225	ALA	C-N-CA	5.25	125.30	119.32
1	C	2145	MET	N-CA-C	5.21	117.37	111.11
1	G	6065	THR	CA-C-N	5.20	125.50	119.47
1	G	6065	THR	C-N-CA	5.20	125.50	119.47
1	A	237	ILE	N-CA-C	5.17	112.27	107.56
1	E	4237	ILE	N-CA-C	5.15	112.24	107.56
1	G	6013	ALA	N-CA-C	-5.12	102.17	110.32
1	A	152	GLU	N-CA-C	-5.12	103.39	110.35
1	E	4101	THR	N-CA-C	5.07	121.61	110.80
1	F	5142	VAL	CA-C-N	5.07	125.30	119.83
1	F	5142	VAL	C-N-CA	5.07	125.30	119.83
1	E	4145	MET	N-CA-C	5.07	116.49	111.07
1	A	201	ILE	N-CA-C	5.05	115.75	108.48
1	D	3012	PHE	N-CA-C	5.00	116.79	109.24

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	2230	0	2234	108	0
1	B	2230	0	2231	107	0
1	C	2230	0	2231	114	0
1	D	2230	0	2231	95	0
1	E	2230	0	2231	104	0
1	F	2230	0	2231	93	0
1	G	2230	0	2231	103	0
1	H	2230	0	2231	115	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
3	A	231	0	0	18	0
3	B	225	0	0	13	0
3	C	226	0	0	14	0
3	D	215	0	0	8	0
3	E	239	0	0	7	0
3	F	226	0	0	9	0
3	G	206	0	0	11	0
3	H	226	0	0	16	0
All	All	19658	0	17851	760	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 21.

All (760) 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:D:3104:VAL:HG22	1:D:3151:ILE:HG22	1.31	1.12
1:E:4125:ALA:HB3	1:E:4129:GLN:HG3	1.31	1.09
1:F:5125:ALA:HB3	1:F:5129:GLN:HG3	1.43	0.98
1:D:3140:TRP:HE1	1:D:3153:ASN:HD22	1.08	0.98
1:E:4104:VAL:HG22	1:E:4151:ILE:HG22	1.46	0.97
1:B:1069:ARG:HB2	3:B:8597:HOH:O	1.65	0.95
1:H:7010:GLU:HG2	1:H:7294:ASN:HD22	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5140:TRP:HE1	1:F:5153:ASN:HD22	1.15	0.94
1:B:1125:ALA:HB3	1:B:1129:GLN:HG3	1.48	0.93
1:F:5104:VAL:HG22	1:F:5151:ILE:HG22	1.48	0.93
1:H:7104:VAL:HG22	1:H:7151:ILE:HG13	1.47	0.93
1:G:6140:TRP:HE1	1:G:6153:ASN:HD22	1.15	0.92
1:H:7085:GLU:O	1:H:7089:LEU:HD23	1.70	0.92
1:B:1208:VAL:HG23	1:B:1209:GLY:H	1.37	0.90
1:A:2:LYS:NZ	1:A:7:GLU:HG2	1.87	0.89
1:G:6246:GLU:HB3	1:H:7145:MET:HE1	1.55	0.89
1:G:6087:GLN:HE21	1:G:6091:ARG:HE	1.20	0.89
1:F:5047:VAL:HG13	1:F:5053:GLU:HG3	1.53	0.89
1:C:2129:GLN:H	1:C:2129:GLN:HE21	1.18	0.88
1:A:203:ALA:O	1:B:1144:MET:HE3	1.72	0.88
1:C:2144:MET:HE3	1:D:3203:ALA:O	1.74	0.88
1:F:5078:HIS:HD2	1:F:5080:SER:H	1.18	0.88
1:H:7119:PHE:HB2	3:H:9558:HOH:O	1.74	0.87
1:C:2087:GLN:HE21	1:C:2091:ARG:HE	1.21	0.87
1:B:1104:VAL:HG22	1:B:1151:ILE:HG13	1.57	0.87
1:G:6078:HIS:HD2	1:G:6080:SER:H	1.18	0.87
1:C:2129:GLN:H	1:C:2129:GLN:NE2	1.74	0.85
1:G:6129:GLN:H	1:G:6129:GLN:HE21	1.21	0.84
1:B:1140:TRP:HE1	1:B:1153:ASN:ND2	1.76	0.83
1:C:2017:ASP:OD1	1:C:2288:LYS:HD3	1.78	0.83
1:H:7129:GLN:H	1:H:7129:GLN:HE21	1.27	0.82
1:E:4281:ASN:HD22	1:E:4283:GLY:H	1.28	0.82
1:E:4127:GLY:H	1:E:4129:GLN:NE2	1.76	0.82
1:G:6169:MET:HG2	1:G:6244:VAL:HG22	1.60	0.81
1:C:2059:LYS:HG2	1:C:2072:TYR:CE2	2.16	0.81
1:E:4117:THR:HG21	1:E:4155:ILE:HD12	1.62	0.81
1:E:4078:HIS:HD2	1:E:4080:SER:H	1.28	0.81
1:G:6140:TRP:HE1	1:G:6153:ASN:ND2	1.77	0.81
1:B:1009:GLU:HB2	1:B:1276:LYS:NZ	1.95	0.80
1:B:1029:ASP:OD1	1:C:2181:LYS:HE3	1.81	0.80
1:B:1078:HIS:HD2	1:B:1080:SER:H	1.28	0.80
1:G:6127:GLY:H	1:G:6129:GLN:HE22	1.30	0.80
1:D:3140:TRP:HE1	1:D:3153:ASN:ND2	1.80	0.80
1:G:6220:THR:HG21	1:H:7143:PRO:O	1.81	0.79
1:C:2078:HIS:HD2	1:C:2080:SER:H	1.29	0.79
1:E:4229:ARG:NH1	1:E:4229:ARG:HB3	1.98	0.79
1:G:6285:LYS:H	1:G:6285:LYS:HD2	1.47	0.79
1:C:2087:GLN:NE2	1:C:2091:ARG:HE	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LYS:HE3	1:A:278:THR:CG2	2.13	0.78
1:F:5085:GLU:O	1:F:5089:LEU:HD23	1.83	0.78
1:A:78:HIS:HD2	1:A:80:SER:H	1.31	0.78
1:A:38:ASN:HD21	1:B:1038:ASN:HD21	1.31	0.78
1:A:47:VAL:HG13	1:A:53:GLU:HG3	1.64	0.78
1:A:276:LYS:HE3	1:A:278:THR:HG21	1.65	0.78
1:H:7129:GLN:H	1:H:7129:GLN:NE2	1.82	0.78
1:G:6129:GLN:H	1:G:6129:GLN:NE2	1.83	0.77
1:E:4038:ASN:HD21	1:F:5038:ASN:HD21	1.30	0.77
1:H:7010:GLU:HG2	1:H:7294:ASN:ND2	1.99	0.77
1:H:7137:ARG:HH21	1:H:7137:ARG:HG3	1.49	0.77
1:E:4127:GLY:H	1:E:4129:GLN:HE22	1.29	0.77
1:C:2085:GLU:O	1:C:2089:LEU:HD23	1.84	0.77
1:H:7153:ASN:HB3	3:H:9558:HOH:O	1.83	0.76
1:A:180:ALA:HB3	3:A:8489:HOH:O	1.84	0.76
1:A:32:TRP:HA	3:A:8879:HOH:O	1.86	0.76
1:E:4143:PRO:O	1:F:5220:THR:HG21	1.85	0.76
1:A:85:GLU:O	1:A:89:LEU:HD13	1.85	0.75
1:G:6166:PHE:CZ	1:G:6247:ILE:HD12	2.21	0.75
1:G:6087:GLN:NE2	1:G:6091:ARG:HE	1.84	0.75
1:E:4154:ASP:HA	3:E:8290:HOH:O	1.86	0.75
1:A:288:LYS:HD3	1:A:288:LYS:O	1.85	0.75
1:E:4094:GLN:HE22	1:F:5048:ILE:CG1	2.00	0.75
1:D:3106:ASN:HB3	1:D:3137:ARG:HH11	1.51	0.74
1:B:1087:GLN:HE21	1:B:1091:ARG:HE	1.35	0.74
1:B:1127:GLY:H	1:B:1129:GLN:NE2	1.85	0.74
1:G:6144:MET:HE3	1:H:7203:ALA:O	1.87	0.74
1:E:4127:GLY:N	1:E:4129:GLN:HE22	1.85	0.74
1:B:1127:GLY:N	1:B:1129:GLN:HE22	1.84	0.74
1:B:1127:GLY:H	1:B:1129:GLN:HE22	1.34	0.74
1:A:59:LYS:HG2	1:A:72:TYR:CE2	2.22	0.74
1:B:1114:LYS:HD3	1:B:1154:ASP:OD2	1.88	0.73
1:A:177:LEU:HD12	3:A:8489:HOH:O	1.88	0.73
1:B:1026:THR:HB	3:B:8597:HOH:O	1.87	0.73
1:B:1129:GLN:NE2	1:B:1129:GLN:H	1.87	0.72
1:F:5052:ALA:HB2	1:F:5087:GLN:HG3	1.70	0.72
1:E:4212:LYS:HD3	1:F:5127:GLY:HA3	1.72	0.72
1:G:6039:GLU:HG3	3:G:8795:HOH:O	1.90	0.72
1:A:9:GLU:HB2	1:A:278:THR:HG22	1.71	0.72
1:A:89:LEU:HD21	1:A:120:LYS:NZ	2.05	0.72
1:A:144:MET:HE3	1:B:1203:ALA:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1017:ASP:HA	3:B:8700:HOH:O	1.88	0.71
1:C:2082:LYS:O	1:C:2086:GLU:HG3	1.90	0.71
1:A:2:LYS:HZ3	1:A:7:GLU:HG2	1.54	0.71
1:B:1127:GLY:CA	1:B:1129:GLN:HE22	2.03	0.71
1:H:7071:GLY:HA3	3:H:8694:HOH:O	1.90	0.71
1:A:94:GLN:HE22	1:B:1048:ILE:CG1	2.04	0.71
1:G:6076:ILE:HD13	3:G:8497:HOH:O	1.91	0.71
1:E:4037:ALA:CA	1:E:4074:ILE:HD11	2.21	0.71
1:D:3078:HIS:HD2	1:D:3080:SER:H	1.38	0.70
1:E:4120:LYS:HD2	3:E:9212:HOH:O	1.92	0.70
1:C:2014:GLU:HG2	1:C:2287:GLY:HA3	1.73	0.70
1:A:138:LYS:HB2	3:A:9236:HOH:O	1.92	0.70
1:E:4037:ALA:CB	1:E:4074:ILE:HD11	2.22	0.70
1:D:3113:GLU:HG2	3:D:8413:HOH:O	1.92	0.70
1:H:7078:HIS:HD2	1:H:7080:SER:H	1.38	0.70
1:C:2143:PRO:O	1:D:3220:THR:HG21	1.92	0.69
1:E:4037:ALA:HB1	1:E:4074:ILE:HD11	1.74	0.69
1:D:3127:GLY:H	1:D:3129:GLN:HE22	1.41	0.69
1:G:6104:VAL:CG1	1:G:6151:ILE:HG23	2.21	0.69
1:F:5122:LYS:HD3	1:F:5129:GLN:HG2	1.74	0.69
1:C:2145:MET:HE2	1:D:3205:GLY:CA	2.23	0.69
1:F:5059:LYS:HG2	1:F:5072:TYR:CE2	2.28	0.69
1:E:4140:TRP:HE1	1:E:4153:ASN:HD22	1.39	0.69
1:C:2061:LYS:O	1:C:2064:GLU:HG2	1.93	0.69
1:A:179:ALA:HA	1:A:271:ILE:HG13	1.74	0.68
1:C:2281:ASN:C	1:C:2281:ASN:HD22	2.01	0.68
1:F:5087:GLN:HE21	1:F:5091:ARG:HE	1.40	0.68
1:E:4009:GLU:HB2	1:E:4278:THR:HG22	1.75	0.68
1:B:1140:TRP:HE1	1:B:1153:ASN:HD22	1.39	0.68
1:A:205:GLY:CA	1:B:1145:MET:HE2	2.24	0.68
1:E:4212:LYS:NZ	1:E:4212:LYS:HB3	2.08	0.68
1:B:1169:MET:HG2	1:B:1244:VAL:HG22	1.76	0.67
1:D:3129:GLN:H	1:D:3129:GLN:HE21	1.40	0.67
1:C:2276:LYS:NZ	1:C:2278:THR:HG21	2.09	0.67
1:H:7255:ASP:O	1:H:7259:GLU:HG3	1.94	0.67
1:A:118:GLY:HA3	1:A:153:ASN:HA	1.77	0.67
1:G:6104:VAL:HG13	1:G:6151:ILE:HG23	1.75	0.67
1:F:5169:MET:HG2	1:F:5244:VAL:HG22	1.77	0.67
1:E:4127:GLY:N	1:E:4129:GLN:NE2	2.42	0.67
1:C:2115:ASP:HB3	3:C:9216:HOH:O	1.94	0.67
1:D:3140:TRP:NE1	1:D:3153:ASN:HD22	1.89	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5140:TRP:HE1	1:F:5153:ASN:ND2	1.91	0.67
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.58	0.66
1:D:3104:VAL:CG2	1:D:3151:ILE:HG22	2.19	0.66
1:A:94:GLN:CD	1:B:1049:MET:HB2	2.20	0.66
1:F:5078:HIS:CD2	1:F:5080:SER:H	2.08	0.66
1:A:203:ALA:C	1:B:1144:MET:HE3	2.21	0.66
1:A:208:VAL:O	1:A:218:ALA:HA	1.94	0.66
1:A:2:LYS:HZ1	1:A:7:GLU:HG2	1.58	0.66
1:G:6085:GLU:O	1:G:6089:LEU:HD23	1.96	0.66
1:D:3062:PRO:HD3	3:D:8787:HOH:O	1.97	0.65
1:E:4009:GLU:CB	1:E:4278:THR:HG22	2.26	0.65
1:A:104:VAL:HG22	1:A:151:ILE:HG22	1.77	0.65
1:E:4037:ALA:HA	1:E:4074:ILE:HD11	1.77	0.65
1:H:7173:GLN:HB3	1:H:7174:PRO:HD3	1.78	0.65
1:A:125:ALA:HB3	1:A:129:GLN:HG2	1.79	0.65
1:E:4127:GLY:CA	1:E:4129:GLN:HE22	2.09	0.65
1:B:1046:SER:OG	1:B:1048:ILE:HG12	1.96	0.65
1:H:7127:GLY:H	1:H:7129:GLN:HE22	1.42	0.65
1:H:7193:VAL:CG1	1:H:7249:ILE:HG23	2.26	0.65
1:A:144:MET:HE3	1:B:1203:ALA:C	2.21	0.64
1:C:2287:GLY:HA2	3:C:9020:HOH:O	1.97	0.64
1:A:277:ILE:HD12	3:A:8708:HOH:O	1.98	0.64
1:A:201:ILE:HD13	3:A:8489:HOH:O	1.98	0.64
1:E:4125:ALA:CB	1:E:4129:GLN:HG3	2.17	0.64
1:E:4229:ARG:HB3	1:E:4229:ARG:HH11	1.62	0.64
1:B:1161:ILE:HG12	3:B:8700:HOH:O	1.98	0.64
1:F:5174:PRO:HD3	1:H:7272:PRO:HG2	1.79	0.64
1:B:1125:ALA:HB2	1:B:1142:VAL:HG13	1.80	0.64
1:H:7179:ALA:HA	1:H:7271:ILE:HG13	1.80	0.64
1:A:277:ILE:HG23	3:A:8708:HOH:O	1.98	0.64
1:A:205:GLY:HA3	1:B:1145:MET:HE2	1.79	0.63
1:F:5018:ILE:HG21	1:F:5162:ALA:HB2	1.80	0.63
1:B:1151:ILE:HG23	3:B:8760:HOH:O	1.98	0.63
1:A:149:PHE:CE2	1:A:151:ILE:HG21	2.34	0.63
1:F:5084:LEU:O	1:F:5088:LEU:HD23	1.98	0.63
1:B:1009:GLU:HB2	1:B:1276:LYS:HZ1	1.63	0.63
1:C:2052:ALA:HB2	1:C:2087:GLN:HG3	1.80	0.63
1:H:7137:ARG:HD3	1:H:7152:GLU:OE1	1.98	0.63
1:F:5193:VAL:HG13	1:F:5249:ILE:HG23	1.80	0.62
1:H:7153:ASN:N	1:H:7153:ASN:HD22	1.97	0.62
1:G:6173:GLN:HB3	1:G:6174:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6129:GLN:HE21	1:G:6129:GLN:N	1.96	0.62
1:H:7290:ILE:C	1:H:7291:ILE:HD12	2.25	0.62
1:C:2276:LYS:HZ3	1:C:2278:THR:HG21	1.63	0.62
1:B:1259:GLU:HG3	3:B:8422:HOH:O	1.99	0.62
1:C:2022:ARG:HB3	1:C:2108:LEU:HG	1.81	0.62
1:F:5286:LEU:N	1:F:5286:LEU:HD22	2.15	0.62
1:B:1127:GLY:N	1:B:1129:GLN:NE2	2.47	0.61
1:C:2144:MET:CE	1:C:2146:GLU:HG2	2.30	0.61
1:C:2094:GLN:CG	1:D:3049:MET:HB3	2.30	0.61
1:C:2129:GLN:HE21	1:C:2129:GLN:N	1.95	0.61
1:A:118:GLY:HA2	1:A:151:ILE:HD12	1.82	0.61
1:G:6014:GLU:HG2	3:G:8421:HOH:O	2.00	0.61
1:B:1125:ALA:CB	1:B:1129:GLN:HG3	2.27	0.61
1:G:6075:GLN:HB2	1:G:6194:ILE:HD13	1.83	0.61
1:A:9:GLU:CB	1:A:278:THR:HG22	2.29	0.61
1:B:1022:ARG:HB3	1:B:1108:LEU:HG	1.81	0.61
1:D:3087:GLN:HE21	1:D:3091:ARG:HE	1.48	0.61
1:G:6012:PHE:HB3	1:G:6292:ASN:HD22	1.66	0.61
1:G:6119:PHE:O	1:G:6122:LYS:HG3	2.01	0.61
1:E:4197:PHE:CG	1:E:4202:VAL:HG22	2.36	0.60
1:E:4232:VAL:CG1	1:E:4235:THR:HB	2.31	0.60
1:B:1193:VAL:HG13	1:B:1249:ILE:HG23	1.82	0.60
1:C:2085:GLU:HG3	1:C:2115:ASP:OD2	2.01	0.60
1:C:2120:LYS:HA	1:C:2120:LYS:HE3	1.83	0.60
1:F:5158:THR:HG22	1:F:5159:ASN:N	2.15	0.60
1:F:5179:ALA:HA	1:F:5271:ILE:HG13	1.84	0.60
1:C:2114:LYS:HG2	1:C:2156:GLY:HA2	1.83	0.60
1:E:4061:LYS:O	1:E:4064:GLU:HG2	2.01	0.60
1:B:1119:PHE:O	1:B:1122:LYS:HG3	2.02	0.60
1:A:282:TYR:HB3	1:A:286:LEU:HD23	1.84	0.60
1:G:6076:ILE:HG21	3:G:8497:HOH:O	2.01	0.60
1:G:6287:GLY:HA3	3:G:8421:HOH:O	2.01	0.60
1:D:3129:GLN:H	1:D:3129:GLN:NE2	1.99	0.60
1:A:78:HIS:CD2	1:A:80:SER:H	2.19	0.59
1:A:173:GLN:HB3	1:A:174:PRO:HD3	1.83	0.59
1:C:2151:ILE:HG13	1:C:2151:ILE:O	2.01	0.59
1:F:5158:THR:HG22	1:F:5159:ASN:H	1.67	0.59
1:G:6205:GLY:CA	1:H:7145:MET:HE2	2.31	0.59
1:D:3017:ASP:OD1	1:D:3289:HIS:HE1	1.85	0.59
1:G:6128:TYR:O	1:G:6130:LYS:HD2	2.02	0.59
1:D:3112:GLU:OE2	1:D:3113:GLU:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4294:ASN:HB2	3:E:8467:HOH:O	2.01	0.59
1:A:197:PHE:CG	1:A:202:VAL:HG22	2.38	0.59
1:G:6022:ARG:HD3	1:G:6107:GLY:O	2.01	0.59
1:A:262:ARG:NH1	1:A:266:LEU:HD11	2.17	0.59
1:E:4045:THR:HG23	3:E:8666:HOH:O	2.02	0.59
1:E:4104:VAL:CG2	1:E:4151:ILE:HG22	2.28	0.59
1:G:6193:VAL:HG13	1:G:6249:ILE:HG23	1.85	0.59
1:C:2173:GLN:HB3	1:C:2174:PRO:HD3	1.85	0.59
1:B:1067:ASP:O	1:C:2270:LYS:HE2	2.02	0.59
1:B:1104:VAL:CG2	1:B:1151:ILE:HG13	2.31	0.59
1:C:2082:LYS:HD2	1:C:2082:LYS:N	2.18	0.59
1:E:4179:ALA:HA	1:E:4271:ILE:HG13	1.84	0.59
1:H:7129:GLN:HE21	1:H:7129:GLN:N	1.99	0.59
1:A:228:ILE:O	1:A:232:VAL:HG23	2.03	0.59
1:B:1272:PRO:HG2	1:D:3174:PRO:HD3	1.85	0.58
1:D:3233:GLU:CD	1:D:3234:GLY:H	2.11	0.58
1:G:6091:ARG:HD2	3:G:8497:HOH:O	2.02	0.58
1:B:1089:LEU:HD21	1:B:1120:LYS:HD2	1.84	0.58
1:H:7052:ALA:HB2	1:H:7087:GLN:HG3	1.84	0.58
1:B:1059:LYS:HB3	3:B:8484:HOH:O	2.02	0.58
1:E:4078:HIS:CD2	1:E:4080:SER:H	2.16	0.58
1:G:6213:TYR:HB2	1:G:6216:LEU:HD23	1.86	0.58
1:C:2094:GLN:HG3	1:D:3049:MET:HB3	1.85	0.58
1:D:3078:HIS:CD2	1:D:3080:SER:H	2.21	0.58
1:G:6104:VAL:HG13	1:G:6151:ILE:HA	1.85	0.58
1:C:2262:ARG:HD2	3:C:9269:HOH:O	2.02	0.58
1:F:5087:GLN:NE2	1:F:5091:ARG:HE	2.02	0.58
1:H:7104:VAL:CG2	1:H:7151:ILE:HG13	2.28	0.58
1:B:1193:VAL:CG1	1:B:1249:ILE:HG23	2.33	0.58
1:F:5046:SER:OG	1:F:5048:ILE:HG12	2.04	0.58
1:G:6140:TRP:NE1	1:G:6153:ASN:HD22	1.93	0.58
1:H:7283:GLY:C	1:H:7285:LYS:H	2.11	0.58
1:C:2149:PHE:CE2	1:C:2151:ILE:HG21	2.39	0.57
1:A:145:MET:HE2	1:B:1205:GLY:CA	2.34	0.57
1:A:281:ASN:HD22	1:A:283:GLY:H	1.52	0.57
1:D:3070:PRO:HA	3:D:8787:HOH:O	2.03	0.57
1:E:4049:MET:HB3	1:F:5094:GLN:CG	2.34	0.57
1:G:6094:GLN:CG	1:H:7049:MET:HB3	2.34	0.57
1:D:3020:ILE:HD12	1:D:3160:GLY:HA3	1.86	0.57
1:H:7236:GLN:HB2	3:H:9278:HOH:O	2.04	0.57
1:A:59:LYS:HD3	3:A:8831:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:THR:HG22	1:B:1124:PHE:CE1	2.40	0.57
1:C:2041:THR:HG21	3:C:8572:HOH:O	2.03	0.57
1:G:6127:GLY:N	1:G:6129:GLN:HE22	2.00	0.57
1:D:3087:GLN:NE2	1:D:3091:ARG:HE	2.02	0.57
1:E:4285:LYS:O	1:E:4286:LEU:HB2	2.05	0.57
1:F:5059:LYS:HG2	1:F:5072:TYR:HE2	1.69	0.57
1:E:4173:GLN:HB3	1:E:4174:PRO:HD3	1.85	0.57
1:G:6046:SER:O	1:G:6050:CYS:HB2	2.03	0.57
1:C:2149:PHE:CE2	1:C:2151:ILE:CG2	2.88	0.57
1:B:1202:VAL:HB	1:B:1246:GLU:HB3	1.86	0.57
1:H:7276:LYS:HE2	1:H:7278:THR:CG2	2.35	0.57
1:B:1087:GLN:NE2	1:B:1091:ARG:HE	2.02	0.56
1:F:5009:GLU:CB	1:F:5278:THR:HG22	2.35	0.56
1:B:1122:LYS:HD2	1:B:1122:LYS:C	2.30	0.56
1:D:3291:ILE:HD12	1:D:3291:ILE:N	2.20	0.56
1:G:6012:PHE:CD1	1:G:6290:ILE:HG23	2.40	0.56
1:G:6193:VAL:CG1	1:G:6249:ILE:HG23	2.35	0.56
1:A:89:LEU:HD21	1:A:120:LYS:HZ3	1.70	0.56
1:G:6169:MET:CE	1:G:6276:LYS:HD3	2.36	0.56
1:A:288:LYS:HD3	1:A:288:LYS:C	2.31	0.56
1:C:2047:VAL:HG21	3:C:8864:HOH:O	2.06	0.56
1:E:4022:ARG:HD3	1:E:4107:GLY:O	2.06	0.56
1:H:7193:VAL:HG12	1:H:7194:ILE:N	2.20	0.56
1:A:149:PHE:CE2	1:A:151:ILE:CG2	2.88	0.56
1:F:5024:LEU:HD13	3:F:8794:HOH:O	2.04	0.56
1:E:4016:PHE:CE1	1:E:4286:LEU:HG	2.40	0.56
1:G:6117:THR:OG1	1:G:6155:ILE:HD12	2.06	0.56
1:B:1190:VAL:HG21	3:B:8422:HOH:O	2.05	0.56
1:E:4129:GLN:NE2	1:E:4129:GLN:H	2.03	0.56
1:F:5282:TYR:CB	1:F:5286:LEU:HD23	2.36	0.56
1:G:6149:PHE:CE2	1:G:6151:ILE:HG12	2.41	0.56
1:A:94:GLN:NE2	1:B:1048:ILE:HG13	2.20	0.55
1:E:4217:LYS:O	1:E:4217:LYS:HD3	2.06	0.55
1:H:7059:LYS:HG2	1:H:7072:TYR:CE2	2.41	0.55
1:A:208:VAL:O	1:A:217:LYS:O	2.24	0.55
1:B:1179:ALA:HA	1:B:1271:ILE:HG13	1.88	0.55
1:B:1281:ASN:HD22	1:B:1283:GLY:H	1.55	0.55
1:E:4131:GLU:OE2	1:E:4138:LYS:HE3	2.06	0.55
1:G:6144:MET:CE	1:G:6146:GLU:HG2	2.36	0.55
1:H:7291:ILE:HD12	1:H:7291:ILE:N	2.22	0.55
1:G:6145:MET:HE2	1:H:7244:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:CG1	1:A:249:ILE:HG23	2.36	0.55
1:A:220:THR:HG23	1:B:1124:PHE:O	2.06	0.55
1:C:2193:VAL:HG13	1:C:2249:ILE:HG23	1.88	0.55
1:B:1173:GLN:HB3	1:B:1174:PRO:HD3	1.89	0.55
1:C:2144:MET:HE2	1:C:2146:GLU:HG2	1.88	0.55
1:H:7138:LYS:HE3	1:H:7153:ASN:HB2	1.89	0.55
1:C:2118:GLY:HA2	1:C:2151:ILE:HD12	1.89	0.55
1:G:6181:LYS:O	1:G:6181:LYS:HD3	2.07	0.55
1:F:5118:GLY:HA2	1:F:5151:ILE:HD12	1.89	0.55
3:C:9023:HOH:O	1:D:3043:PHE:HD2	1.89	0.54
1:C:2197:PHE:CG	1:C:2202:VAL:HG22	2.42	0.54
1:G:6094:GLN:HG3	1:H:7049:MET:HB3	1.89	0.54
1:E:4180:ALA:O	1:E:4184:VAL:HG23	2.08	0.54
1:G:6078:HIS:CD2	1:G:6080:SER:H	2.11	0.54
1:H:7022:ARG:HB3	1:H:7108:LEU:HG	1.89	0.54
1:C:2145:MET:HE2	1:D:3205:GLY:N	2.22	0.54
1:F:5149:PHE:CE2	1:F:5151:ILE:CG2	2.91	0.54
1:G:6012:PHE:HB3	1:G:6292:ASN:ND2	2.23	0.54
1:H:7193:VAL:HG11	1:H:7249:ILE:HG23	1.89	0.54
1:C:2018:ILE:HG21	1:C:2162:ALA:HB2	1.88	0.54
1:C:2047:VAL:HG22	1:C:2047:VAL:O	2.07	0.54
1:D:3213:TYR:HB3	1:D:3215:PHE:CE1	2.42	0.54
1:E:4029:ASP:HB2	1:H:7185:ASP:OD2	2.06	0.54
1:E:4022:ARG:HB3	1:E:4108:LEU:HG	1.89	0.54
1:E:4094:GLN:NE2	1:F:5048:ILE:CG1	2.69	0.54
1:G:6022:ARG:CB	1:G:6108:LEU:HG	2.37	0.54
1:E:4197:PHE:CD2	1:E:4202:VAL:HG22	2.43	0.54
1:C:2138:LYS:HG2	3:C:8391:HOH:O	2.08	0.53
1:C:2198:PRO:HG3	1:D:3039:GLU:HG2	1.89	0.53
1:F:5029:ASP:OD1	1:G:6181:LYS:HD2	2.08	0.53
1:G:6291:ILE:HD12	1:G:6291:ILE:N	2.22	0.53
1:H:7221:ASN:C	1:H:7221:ASN:HD22	2.15	0.53
1:B:1078:HIS:CD2	1:B:1080:SER:H	2.17	0.53
1:C:2120:LYS:HZ1	1:C:2123:PHE:HE2	1.55	0.53
1:B:1208:VAL:HG23	1:B:1209:GLY:N	2.15	0.53
1:D:3046:SER:OG	1:D:3048:ILE:HD13	2.08	0.53
1:D:3173:GLN:HB3	1:D:3174:PRO:HD3	1.91	0.53
1:D:3210:ALA:HB3	1:D:3213:TYR:O	2.08	0.53
1:D:3290:ILE:C	1:D:3291:ILE:HD12	2.33	0.53
1:F:5067:ASP:OD1	1:F:5069:ARG:HD3	2.08	0.53
1:G:6122:LYS:HD2	1:G:6122:LYS:C	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2049:MET:HB3	1:D:3094:GLN:CG	2.39	0.53
1:F:5208:VAL:O	1:F:5218:ALA:HA	2.07	0.53
1:F:5282:TYR:HB3	1:F:5286:LEU:HD23	1.89	0.53
1:B:1017:ASP:CG	1:B:1289:HIS:HE1	2.17	0.53
1:C:2049:MET:HB3	1:D:3094:GLN:HG3	1.90	0.53
1:C:2221:ASN:HD21	1:C:2223:LYS:NZ	2.07	0.53
1:E:4037:ALA:HA	1:E:4074:ILE:CD1	2.39	0.53
1:C:2285:LYS:O	1:C:2286:LEU:HB2	2.09	0.53
1:D:3238:PRO:HG2	1:D:3241:VAL:CG2	2.38	0.53
1:E:4236:GLN:O	1:E:4238:PRO:HD3	2.09	0.53
1:G:6056:ILE:N	1:G:6056:ILE:HD12	2.24	0.53
1:A:145:MET:HE2	1:B:1205:GLY:N	2.24	0.53
1:F:5185:ASP:OD2	1:G:6029:ASP:HB2	2.09	0.53
1:H:7001:MET:HB2	1:H:7294:ASN:ND2	2.24	0.53
1:D:3288:LYS:HD3	1:D:3289:HIS:CE1	2.43	0.52
1:E:4214:LYS:C	1:E:4216:LEU:H	2.16	0.52
1:F:5056:ILE:N	1:F:5056:ILE:HD12	2.24	0.52
1:F:5255:ASP:OD2	3:F:9786:HOH:O	2.19	0.52
1:B:1097:LEU:HD23	1:B:1097:LEU:C	2.34	0.52
1:B:1285:LYS:C	1:B:1286:LEU:HD12	2.34	0.52
1:A:138:LYS:HD3	3:A:9528:HOH:O	2.09	0.52
1:A:286:LEU:N	1:A:286:LEU:HD22	2.23	0.52
1:D:3046:SER:O	1:D:3050:CYS:HB2	2.09	0.52
1:E:4117:THR:HB	3:E:8333:HOH:O	2.09	0.52
1:E:4212:LYS:HB3	1:E:4212:LYS:HZ3	1.72	0.52
1:F:5171:GLU:O	1:F:5242:LYS:HE3	2.08	0.52
1:A:97:LEU:C	1:A:97:LEU:HD23	2.35	0.52
1:B:1027:GLY:N	3:B:8597:HOH:O	2.42	0.52
1:F:5208:VAL:O	1:F:5217:LYS:O	2.28	0.52
1:G:6017:ASP:OD1	1:G:6289:HIS:HE1	1.93	0.52
1:H:7193:VAL:CG1	1:H:7194:ILE:N	2.72	0.52
1:D:3056:ILE:N	1:D:3056:ILE:HD12	2.23	0.52
1:E:4094:GLN:NE2	1:F:5048:ILE:HG13	2.24	0.52
1:E:4217:LYS:HD3	1:E:4217:LYS:C	2.35	0.52
1:C:2221:ASN:ND2	1:C:2223:LYS:NZ	2.57	0.52
1:C:2059:LYS:HB2	3:C:9156:HOH:O	2.10	0.52
1:A:193:VAL:HG13	1:A:249:ILE:HG23	1.92	0.52
1:H:7137:ARG:HH21	1:H:7137:ARG:CG	2.19	0.52
1:H:7197:PHE:CD2	1:H:7202:VAL:HG22	2.45	0.52
1:G:6193:VAL:HG23	1:G:6256:ALA:HB1	1.91	0.52
1:G:6253:ASN:O	1:G:6257:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:ASN:OD1	1:B:1270:LYS:HE3	2.10	0.52
1:F:5097:LEU:HD23	1:F:5097:LEU:C	2.35	0.52
1:H:7202:VAL:HG21	1:H:7248:VAL:HG23	1.91	0.52
1:C:2145:MET:HE2	1:D:3205:GLY:HA3	1.91	0.51
1:F:5173:GLN:HB3	1:F:5174:PRO:HD3	1.91	0.51
1:G:6104:VAL:HG11	1:G:6151:ILE:HG23	1.91	0.51
1:C:2205:GLY:CA	1:D:3145:MET:HE2	2.39	0.51
1:C:2212:LYS:HD3	1:D:3127:GLY:HA3	1.91	0.51
1:D:3001:MET:SD	1:D:3294:ASN:HA	2.51	0.51
1:D:3051:PRO:HG2	1:D:3091:ARG:NH2	2.24	0.51
1:H:7283:GLY:O	1:H:7285:LYS:N	2.42	0.51
1:C:2213:TYR:CB	1:C:2216:LEU:HD23	2.39	0.51
1:C:2215:PHE:CD1	1:C:2216:LEU:HD22	2.45	0.51
1:D:3202:VAL:HB	1:D:3246:GLU:HB3	1.93	0.51
1:E:4016:PHE:HE1	1:E:4286:LEU:HG	1.75	0.51
1:E:4145:MET:HE1	1:F:5246:GLU:HB3	1.92	0.51
1:F:5285:LYS:C	1:F:5286:LEU:HD22	2.35	0.51
1:C:2015:ALA:HB3	1:C:2289:HIS:HB2	1.92	0.51
1:C:2097:LEU:HD23	1:C:2097:LEU:O	2.10	0.51
1:F:5197:PHE:CG	1:F:5202:VAL:HG22	2.45	0.51
1:D:3106:ASN:O	1:D:3137:ARG:NH1	2.43	0.51
1:B:1122:LYS:HD3	1:B:1129:GLN:HG2	1.93	0.51
1:C:2052:ALA:HB1	1:C:2077:CYS:O	2.10	0.51
1:C:2285:LYS:O	1:C:2286:LEU:CB	2.59	0.51
1:H:7262:ARG:HD2	3:H:8143:HOH:O	2.10	0.51
1:D:3082:LYS:O	1:D:3086:GLU:HB2	2.11	0.51
1:C:2097:LEU:HD23	1:C:2097:LEU:C	2.36	0.51
1:F:5059:LYS:HG3	3:F:8996:HOH:O	2.11	0.51
1:A:1:MET:HE1	1:A:294:ASN:HA	1.92	0.50
1:A:232:VAL:O	1:A:233:GLU:CB	2.59	0.50
1:C:2059:LYS:HE2	1:C:2072:TYR:OH	2.12	0.50
1:G:6193:VAL:CG1	1:G:6194:ILE:N	2.73	0.50
1:H:7017:ASP:OD1	1:H:7288:LYS:HE2	2.11	0.50
1:H:7290:ILE:N	1:H:7290:ILE:HD12	2.26	0.50
1:D:3014:GLU:HG2	1:D:3287:GLY:HA3	1.94	0.50
1:F:5197:PHE:CD2	1:F:5202:VAL:HG22	2.46	0.50
1:G:6095:CYS:SG	3:G:8795:HOH:O	2.60	0.50
1:H:7161:ILE:HG22	3:H:8809:HOH:O	2.10	0.50
1:B:1197:PHE:HB3	1:B:1198:PRO:HD2	1.93	0.50
1:F:5129:GLN:CD	1:F:5129:GLN:H	2.19	0.50
1:H:7118:GLY:HA3	1:H:7152:GLU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7197:PHE:CG	1:H:7202:VAL:HG22	2.47	0.50
1:A:286:LEU:HD22	1:A:286:LEU:H	1.76	0.50
1:F:5060:ALA:HB2	3:F:8794:HOH:O	2.11	0.50
1:A:144:MET:HE3	1:B:1204:SER:HA	1.93	0.50
1:D:3228:ILE:O	1:D:3232:VAL:HG23	2.12	0.50
1:G:6094:GLN:HE22	1:H:7048:ILE:CG2	2.24	0.50
1:G:6294:ASN:HB2	3:G:8361:HOH:O	2.12	0.50
1:A:295:GLU:N	3:A:9367:HOH:O	2.44	0.50
1:D:3057:GLU:HG2	1:D:3058:ILE:HG23	1.93	0.50
1:A:94:GLN:HE22	1:B:1048:ILE:HG13	1.72	0.49
1:D:3061:LYS:O	1:D:3064:GLU:HG3	2.12	0.49
1:F:5009:GLU:HB2	1:F:5278:THR:HG22	1.94	0.49
1:G:6042:GLY:O	1:G:6043:PHE:C	2.54	0.49
1:H:7201:ILE:HG21	3:H:8534:HOH:O	2.11	0.49
1:C:2213:TYR:HB2	1:C:2216:LEU:HD23	1.94	0.49
1:A:151:ILE:HG13	1:A:151:ILE:O	2.12	0.49
1:H:7015:ALA:HB3	1:H:7289:HIS:HB2	1.93	0.49
1:H:7119:PHE:O	1:H:7122:LYS:HG3	2.12	0.49
1:B:1193:VAL:CG1	1:B:1194:ILE:N	2.75	0.49
1:C:2131:GLU:HG3	3:C:8391:HOH:O	2.11	0.49
1:D:3170:ALA:HB3	1:D:3176:ALA:HB2	1.94	0.49
1:E:4221:ASN:HD22	1:E:4221:ASN:C	2.19	0.49
1:G:6094:GLN:HE22	1:H:7048:ILE:HG22	1.77	0.49
1:H:7009:GLU:HB3	1:H:7278:THR:HG22	1.94	0.49
1:H:7170:ALA:HA	1:H:7275:VAL:HG23	1.95	0.49
1:B:1052:ALA:HB2	1:B:1087:GLN:HG3	1.93	0.49
1:G:6145:MET:HE1	1:H:7246:GLU:HB2	1.93	0.49
1:H:7138:LYS:O	1:H:7138:LYS:HG3	2.13	0.49
1:A:145:MET:HE2	1:B:1205:GLY:HA3	1.93	0.49
1:G:6144:MET:HE2	1:G:6146:GLU:HG2	1.94	0.49
3:G:8795:HOH:O	1:H:7043:PHE:HA	2.12	0.49
1:D:3026:THR:O	1:D:3102:THR:HA	2.13	0.49
1:F:5009:GLU:HB3	1:F:5278:THR:HG22	1.94	0.49
1:A:221:ASN:C	1:A:221:ASN:HD22	2.21	0.49
1:F:5114:LYS:HG2	1:F:5156:GLY:HA2	1.93	0.49
1:G:6169:MET:HE3	1:G:6276:LYS:HD3	1.93	0.49
1:B:1144:MET:HE2	1:B:1146:GLU:HG2	1.94	0.48
1:B:1193:VAL:HG12	1:B:1194:ILE:N	2.28	0.48
1:E:4052:ALA:HB2	1:E:4087:GLN:HG3	1.95	0.48
1:G:6281:ASN:C	1:G:6281:ASN:HD22	2.21	0.48
1:H:7001:MET:HB2	1:H:7294:ASN:HD21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7233:GLU:HG2	1:H:7234:GLY:N	2.28	0.48
1:H:7286:LEU:HA	3:H:8769:HOH:O	2.13	0.48
1:C:2108:LEU:O	1:C:2114:LYS:NZ	2.46	0.48
1:A:138:LYS:HA	3:A:8756:HOH:O	2.12	0.48
1:E:4042:GLY:O	1:E:4043:PHE:C	2.56	0.48
1:E:4232:VAL:HG13	1:E:4235:THR:HB	1.94	0.48
1:F:5116:ASP:HA	1:F:5154:ASP:OD1	2.14	0.48
1:G:6052:ALA:HB2	1:G:6087:GLN:HG3	1.94	0.48
1:A:22:ARG:HB3	1:A:108:LEU:HG	1.95	0.48
1:A:213:TYR:O	1:A:216:LEU:HB2	2.13	0.48
1:D:3042:GLY:O	1:D:3043:PHE:C	2.56	0.48
1:D:3197:PHE:CG	1:D:3202:VAL:HG22	2.48	0.48
1:G:6204:SER:O	1:H:7145:MET:HG3	2.14	0.48
1:H:7009:GLU:CB	1:H:7278:THR:HG22	2.43	0.48
1:H:7113:GLU:HB2	1:H:7157:TYR:CZ	2.48	0.48
1:B:1026:THR:O	1:B:1102:THR:HA	2.13	0.48
1:C:2221:ASN:C	1:C:2221:ASN:HD22	2.22	0.48
1:H:7127:GLY:N	1:H:7129:GLN:HE22	2.10	0.48
1:C:2149:PHE:CZ	1:C:2151:ILE:CG2	2.97	0.48
1:E:4026:THR:O	1:E:4102:THR:HA	2.14	0.48
1:G:6067:ASP:OD1	1:G:6069:ARG:HD2	2.14	0.48
1:A:193:VAL:CG1	1:A:194:ILE:N	2.77	0.48
1:D:3030:TYR:CE2	1:D:3059:LYS:HG3	2.48	0.48
1:D:3127:GLY:N	1:D:3129:GLN:HE22	2.08	0.48
1:B:1067:ASP:OD1	1:B:1069:ARG:HD3	2.14	0.48
1:C:2078:HIS:CD2	1:C:2080:SER:H	2.19	0.48
1:C:2257:ILE:HG21	1:C:2291:ILE:HD11	1.96	0.48
1:B:1009:GLU:CB	1:B:1278:THR:HG22	2.43	0.48
1:B:1197:PHE:CG	1:B:1202:VAL:HG22	2.49	0.48
1:C:2029:ASP:HA	1:C:2070:PRO:CG	2.44	0.48
1:C:2114:LYS:HE3	3:C:9442:HOH:O	2.13	0.48
1:H:7112:GLU:C	1:H:7112:GLU:CD	2.81	0.48
1:H:7132:VAL:HG12	1:H:7133:GLU:N	2.29	0.48
1:A:52:ALA:HB2	1:A:87:GLN:HG3	1.96	0.47
1:C:2120:LYS:HA	1:C:2120:LYS:CE	2.44	0.47
1:E:4046:SER:O	1:E:4050:CYS:HB2	2.13	0.47
1:F:5193:VAL:CG1	1:F:5249:ILE:HG23	2.44	0.47
1:G:6197:PHE:CD2	1:G:6202:VAL:HG22	2.48	0.47
1:H:7058:ILE:HG13	1:H:7059:LYS:N	2.29	0.47
1:A:295:GLU:HG3	3:A:9367:HOH:O	2.13	0.47
1:C:2221:ASN:ND2	1:C:2223:LYS:HZ2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6058:ILE:HG13	1:G:6059:LYS:N	2.30	0.47
1:D:3169:MET:HG2	1:D:3244:VAL:HG22	1.97	0.47
1:B:1097:LEU:HD23	1:B:1097:LEU:O	2.14	0.47
1:D:3197:PHE:HB3	1:D:3198:PRO:HD2	1.97	0.47
1:E:4009:GLU:HB3	1:E:4278:THR:HG22	1.97	0.47
1:E:4058:ILE:C	1:E:4058:ILE:HD12	2.39	0.47
1:G:6022:ARG:HB3	1:G:6108:LEU:HG	1.95	0.47
1:H:7140:TRP:CD1	1:H:7153:ASN:ND2	2.83	0.47
1:B:1113:GLU:HG2	3:B:8360:HOH:O	2.13	0.47
1:C:2043:PHE:HB3	3:C:9023:HOH:O	2.15	0.47
1:D:3051:PRO:HG2	1:D:3091:ARG:HH21	1.80	0.47
1:E:4041:THR:HG23	1:E:4074:ILE:HD13	1.97	0.47
1:E:4291:ILE:HD12	1:E:4291:ILE:N	2.29	0.47
1:A:168:ILE:HG12	3:A:8708:HOH:O	2.14	0.47
1:C:2193:VAL:CG1	1:C:2249:ILE:HG23	2.45	0.47
1:E:4149:PHE:CZ	1:E:4151:ILE:HG23	2.50	0.47
1:C:2193:VAL:CG1	1:C:2194:ILE:N	2.78	0.47
1:H:7113:GLU:H	1:H:7113:GLU:CD	2.21	0.47
1:C:2213:TYR:CE1	1:D:3123:PHE:HD1	2.33	0.47
1:E:4171:GLU:O	1:E:4242:LYS:HD2	2.15	0.47
1:E:4193:VAL:HG13	1:E:4249:ILE:HG23	1.97	0.47
1:H:7137:ARG:HG3	1:H:7137:ARG:NH2	2.25	0.47
1:D:3125:ALA:HB3	1:D:3129:GLN:HB3	1.97	0.46
1:D:3193:VAL:HG13	1:D:3194:ILE:N	2.30	0.46
1:F:5149:PHE:CE2	1:F:5151:ILE:HG21	2.50	0.46
1:B:1058:ILE:HG22	1:B:1188:SER:O	2.15	0.46
1:G:6022:ARG:HB2	1:G:6108:LEU:HG	1.97	0.46
1:B:1009:GLU:HB3	1:B:1278:THR:HG22	1.97	0.46
1:G:6197:PHE:CG	1:G:6202:VAL:HG22	2.50	0.46
1:F:5009:GLU:HG3	3:F:9458:HOH:O	2.15	0.46
1:E:4078:HIS:CD2	1:E:4083:GLY:HA3	2.51	0.46
1:C:2289:HIS:C	1:C:2290:ILE:HD12	2.41	0.46
1:E:4129:GLN:H	1:E:4129:GLN:CD	2.23	0.46
1:C:2001:MET:SD	1:C:2294:ASN:HA	2.56	0.46
1:E:4094:GLN:HE22	1:F:5048:ILE:HG13	1.79	0.46
1:E:4181:LYS:HE2	3:H:8376:HOH:O	2.16	0.46
1:E:4208:VAL:HG23	1:E:4282:TYR:CE2	2.50	0.46
1:A:94:GLN:HE22	1:B:1048:ILE:HG12	1.80	0.46
1:A:232:VAL:O	1:A:233:GLU:HB2	2.14	0.46
1:F:5253:ASN:ND2	1:F:5256:ALA:H	2.14	0.46
1:H:7223:LYS:HB3	3:H:9278:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7181:LYS:O	1:H:7181:LYS:HD3	2.17	0.45
1:A:292:ASN:CB	3:A:9367:HOH:O	2.65	0.45
1:E:4030:TYR:CE2	1:E:4059:LYS:HG3	2.51	0.45
1:E:4049:MET:HB3	1:F:5094:GLN:HG3	1.98	0.45
1:F:5018:ILE:HD12	1:F:5079:MET:HE2	1.98	0.45
1:A:197:PHE:CD2	1:A:202:VAL:HG22	2.50	0.45
1:A:292:ASN:HB2	3:A:9367:HOH:O	2.15	0.45
1:F:5068:GLY:HA3	1:G:6270:LYS:HE3	1.98	0.45
1:F:5125:ALA:CB	1:F:5129:GLN:HG3	2.30	0.45
1:G:6288:LYS:HE2	1:G:6289:HIS:CE1	2.52	0.45
3:G:8795:HOH:O	1:H:7043:PHE:N	2.49	0.45
1:A:97:LEU:HD23	1:A:97:LEU:O	2.17	0.45
1:C:2008:VAL:HG22	1:C:2277:ILE:HB	1.98	0.45
1:C:2078:HIS:CD2	1:C:2083:GLY:HA3	2.52	0.45
1:C:2114:LYS:HG2	1:C:2156:GLY:CA	2.46	0.45
1:D:3061:LYS:HA	3:D:8787:HOH:O	2.16	0.45
1:F:5193:VAL:CG1	1:F:5194:ILE:N	2.79	0.45
3:B:8836:HOH:O	1:F:5214:LYS:HE3	2.15	0.45
1:E:4119:PHE:O	1:E:4122:LYS:HG3	2.17	0.45
1:E:4122:LYS:HD3	1:E:4129:GLN:HG2	1.99	0.45
1:A:62:PRO:HG3	1:A:70:PRO:HG3	1.98	0.45
1:A:286:LEU:H	1:A:286:LEU:CD2	2.30	0.45
1:C:2145:MET:HG3	1:D:3204:SER:O	2.16	0.45
1:C:2191:GLU:HB3	3:E:8926:HOH:O	2.17	0.45
1:C:2212:LYS:HE2	1:C:2212:LYS:HB3	1.83	0.45
1:G:6047:VAL:O	1:G:6047:VAL:HG22	2.17	0.45
1:A:137:ARG:HG2	1:A:137:ARG:NH1	2.28	0.45
1:E:4290:ILE:N	1:E:4290:ILE:HD12	2.32	0.45
1:G:6259:GLU:O	1:G:6259:GLU:HG3	2.17	0.45
1:A:293:LEU:HD12	1:A:293:LEU:H	1.81	0.45
1:B:1129:GLN:H	1:B:1129:GLN:CD	2.24	0.45
1:D:3024:LEU:HG	3:D:8777:HOH:O	2.17	0.45
1:D:3026:THR:HG23	3:D:8777:HOH:O	2.17	0.45
1:G:6017:ASP:OD1	1:G:6289:HIS:CE1	2.70	0.45
1:G:6285:LYS:H	1:G:6285:LYS:CD	2.25	0.45
1:H:7018:ILE:HG21	1:H:7162:ALA:HB2	1.99	0.45
1:H:7113:GLU:HG3	1:H:7157:TYR:CE1	2.51	0.45
1:A:180:ALA:HB1	1:A:247:ILE:HD11	1.98	0.44
1:C:2042:GLY:O	1:C:2043:PHE:C	2.60	0.44
1:C:2149:PHE:CZ	1:C:2151:ILE:HG22	2.52	0.44
1:E:4094:GLN:HE22	1:F:5048:ILE:HG12	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5100:PRO:C	1:F:5101:THR:HG23	2.41	0.44
1:G:6193:VAL:HG12	1:G:6194:ILE:N	2.30	0.44
1:C:2145:MET:HE1	1:D:3246:GLU:HB3	1.99	0.44
1:C:2290:ILE:HD12	1:C:2290:ILE:N	2.32	0.44
1:E:4193:VAL:CG1	1:E:4194:ILE:N	2.80	0.44
1:H:7097:LEU:HD23	1:H:7097:LEU:C	2.43	0.44
1:A:12:PHE:HB3	1:A:292:ASN:OD1	2.18	0.44
1:C:2276:LYS:HZ3	1:C:2278:THR:CG2	2.30	0.44
1:G:6049:MET:HB3	1:H:7094:GLN:CG	2.47	0.44
1:E:4145:MET:HE2	1:F:5205:GLY:CA	2.47	0.44
1:B:1210:ALA:HB3	1:B:1213:TYR:O	2.17	0.44
1:C:2183:ALA:O	1:C:2187:ILE:HG13	2.18	0.44
1:D:3256:ALA:HB1	3:D:8775:HOH:O	2.17	0.44
1:H:7113:GLU:HG2	1:H:7157:TYR:O	2.17	0.44
1:A:59:LYS:HG3	3:A:8651:HOH:O	2.18	0.44
1:B:1129:GLN:C	1:B:1130:LYS:HG3	2.43	0.44
1:E:4167:PHE:N	1:E:4167:PHE:CD2	2.86	0.44
1:F:5224:PHE:O	1:F:5226:PRO:HD3	2.18	0.44
1:C:2144:MET:HE3	1:C:2146:GLU:HG2	1.99	0.44
1:B:1140:TRP:NE1	1:B:1153:ASN:HD22	2.12	0.44
1:B:1161:ILE:HA	3:B:8700:HOH:O	2.18	0.44
1:C:2082:LYS:N	1:C:2082:LYS:CD	2.80	0.44
1:D:3238:PRO:HG2	1:D:3241:VAL:HG23	2.00	0.44
1:H:7283:GLY:C	1:H:7285:LYS:N	2.76	0.44
1:A:59:LYS:HG2	1:A:72:TYR:HE2	1.81	0.44
1:F:5170:ALA:HB3	1:F:5176:ALA:HB2	2.00	0.44
1:F:5189:ASP:HB2	3:F:9661:HOH:O	2.17	0.44
1:H:7193:VAL:CG1	1:H:7249:ILE:CG2	2.96	0.44
1:H:7138:LYS:HG2	3:H:9596:HOH:O	2.18	0.43
1:B:1286:LEU:HD12	1:B:1286:LEU:N	2.33	0.43
1:C:2270:LYS:NZ	3:C:8567:HOH:O	2.50	0.43
1:F:5257:ILE:HG21	1:F:5291:ILE:HD11	2.00	0.43
1:H:7112:GLU:CD	1:H:7113:GLU:N	2.76	0.43
1:H:7293:LEU:HD12	1:H:7293:LEU:N	2.33	0.43
1:B:1138:LYS:HZ2	1:B:1153:ASN:HD22	1.67	0.43
1:D:3110:ASP:O	1:D:3111:ALA:HB3	2.17	0.43
1:H:7286:LEU:HD23	1:H:7286:LEU:O	2.18	0.43
1:A:149:PHE:CZ	1:A:151:ILE:CG2	3.01	0.43
1:B:1046:SER:O	1:B:1050:CYS:HB2	2.19	0.43
1:B:1118:GLY:HA3	1:B:1152:GLU:O	2.18	0.43
1:C:2239:ALA:HB1	3:C:8574:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3292:ASN:HB3	1:D:3294:ASN:OD1	2.18	0.43
1:E:4062:PRO:HB3	1:E:4068:GLY:O	2.18	0.43
1:F:5149:PHE:CZ	1:F:5151:ILE:CG2	3.02	0.43
1:G:6067:ASP:OD1	1:G:6069:ARG:CD	2.66	0.43
1:H:7193:VAL:HG23	1:H:7256:ALA:HB1	2.01	0.43
1:A:145:MET:HE2	1:B:1204:SER:C	2.43	0.43
1:C:2022:ARG:HD3	1:C:2107:GLY:O	2.18	0.43
1:C:2029:ASP:HA	1:C:2070:PRO:HG3	2.01	0.43
1:C:2205:GLY:N	1:D:3145:MET:HE2	2.34	0.43
1:H:7193:VAL:HG11	1:H:7249:ILE:CG2	2.48	0.43
1:D:3011:THR:O	1:D:3293:LEU:HD13	2.19	0.43
1:F:5042:GLY:O	1:F:5043:PHE:C	2.61	0.43
1:A:276:LYS:HE2	3:A:9285:HOH:O	2.19	0.43
1:B:1197:PHE:CD2	1:B:1202:VAL:HG22	2.54	0.43
1:D:3122:LYS:HD3	1:D:3129:GLN:HG3	2.00	0.43
1:E:4222:GLU:CD	1:E:4222:GLU:H	2.26	0.43
1:F:5285:LYS:HB2	1:F:5286:LEU:HD22	2.01	0.43
1:F:5286:LEU:N	1:F:5286:LEU:CD2	2.82	0.43
1:G:6118:GLY:HA3	1:G:6152:GLU:O	2.18	0.43
1:D:3075:GLN:HB2	1:D:3194:ILE:HD13	2.00	0.43
1:H:7137:ARG:CG	1:H:7137:ARG:NH2	2.80	0.43
1:B:1015:ALA:HB1	1:B:1162:ALA:O	2.18	0.43
1:D:3083:GLY:O	1:D:3086:GLU:HB3	2.18	0.43
1:D:3132:VAL:HG12	3:D:8287:HOH:O	2.18	0.43
1:D:3233:GLU:CD	1:D:3234:GLY:N	2.77	0.43
1:E:4185:ASP:OD2	1:H:7029:ASP:HB2	2.19	0.43
1:E:4208:VAL:HG23	1:E:4282:TYR:HE2	1.82	0.43
1:G:6293:LEU:HD12	1:G:6293:LEU:N	2.34	0.43
1:H:7233:GLU:HG2	1:H:7234:GLY:H	1.83	0.43
1:A:29:ASP:HB2	1:D:3185:ASP:OD2	2.18	0.43
1:C:2197:PHE:CD2	1:C:2202:VAL:HG22	2.54	0.43
1:F:5024:LEU:HD12	1:F:5025:ILE:N	2.34	0.43
1:G:6169:MET:HE1	3:G:8925:HOH:O	2.19	0.43
1:E:4293:LEU:HD12	1:E:4293:LEU:N	2.34	0.42
1:H:7042:GLY:O	1:H:7043:PHE:C	2.61	0.42
1:C:2017:ASP:CG	1:C:2289:HIS:HE1	2.27	0.42
1:E:4117:THR:CG2	1:E:4155:ILE:HD12	2.43	0.42
1:F:5114:LYS:HG2	1:F:5156:GLY:CA	2.49	0.42
1:A:26:THR:O	1:A:102:THR:HA	2.18	0.42
1:B:1208:VAL:O	1:B:1218:ALA:HA	2.19	0.42
1:D:3012:PHE:CD1	1:D:3290:ILE:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4232:VAL:HG11	1:E:4235:THR:HB	2.00	0.42
1:G:6181:LYS:HD3	1:G:6181:LYS:C	2.44	0.42
1:G:6205:GLY:HA3	1:H:7145:MET:HE2	2.00	0.42
1:H:7014:GLU:HB2	1:H:7281:ASN:HA	2.01	0.42
1:H:7089:LEU:HD21	3:H:9170:HOH:O	2.19	0.42
1:G:6075:GLN:HB2	1:G:6194:ILE:HG21	2.02	0.42
1:D:3016:PHE:HE1	1:D:3286:LEU:O	2.03	0.42
1:F:5270:LYS:HE3	1:G:6068:GLY:O	2.18	0.42
1:G:6014:GLU:OE2	1:G:6282:TYR:HB2	2.19	0.42
1:G:6169:MET:HG2	1:G:6244:VAL:CG2	2.41	0.42
1:H:7051:PRO:HB2	1:H:7087:GLN:NE2	2.34	0.42
1:A:177:LEU:HD13	1:B:1100:PRO:HB3	2.02	0.42
1:A:193:VAL:HG12	1:A:194:ILE:N	2.34	0.42
1:B:1138:LYS:NZ	1:B:1153:ASN:HD22	2.17	0.42
1:F:5158:THR:CG2	1:F:5159:ASN:N	2.83	0.42
1:G:6032:TRP:CH2	1:H:7177:LEU:HD11	2.54	0.42
1:H:7114:LYS:HE3	3:H:8998:HOH:O	2.19	0.42
1:H:7180:ALA:HB3	3:H:8534:HOH:O	2.20	0.42
1:D:3131:GLU:HG2	1:D:3140:TRP:CZ3	2.55	0.42
1:D:3193:VAL:CG1	1:D:3194:ILE:N	2.79	0.42
1:F:5097:LEU:HD23	1:F:5097:LEU:O	2.20	0.42
1:H:7085:GLU:HG3	1:H:7115:ASP:OD1	2.20	0.42
1:A:12:PHE:CD1	1:A:290:ILE:HG23	2.54	0.42
1:A:131:GLU:HG3	1:A:140:TRP:CZ3	2.54	0.42
1:C:2045:THR:HG21	1:C:2198:PRO:HD3	2.02	0.42
1:D:3081:LYS:NZ	1:D:3081:LYS:CB	2.83	0.42
1:D:3197:PHE:CD2	1:D:3202:VAL:HG22	2.55	0.42
1:E:4058:ILE:HD11	1:E:4073:TYR:CD1	2.55	0.42
1:E:4094:GLN:HE22	1:F:5048:ILE:CD1	2.33	0.42
1:B:1010:GLU:HB3	1:B:1294:ASN:OD1	2.20	0.42
1:H:7087:GLN:HE21	1:H:7091:ARG:HE	1.68	0.42
1:H:7138:LYS:HE3	1:H:7153:ASN:CB	2.50	0.42
1:B:1057:GLU:O	1:B:1058:ILE:HG23	2.20	0.41
1:B:1254:ALA:O	1:B:1258:LYS:HG3	2.19	0.41
1:C:2293:LEU:HD12	1:C:2293:LEU:N	2.35	0.41
1:D:3129:GLN:HE21	1:D:3129:GLN:N	2.14	0.41
1:E:4057:GLU:HG2	1:E:4058:ILE:HG23	2.02	0.41
1:E:4254:ALA:O	1:E:4258:LYS:HG3	2.20	0.41
1:F:5062:PRO:HG3	1:F:5070:PRO:HG3	2.01	0.41
1:G:6045:THR:HG21	1:G:6198:PRO:HD3	2.02	0.41
1:A:282:TYR:CB	1:A:286:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD12	1:A:293:LEU:N	2.35	0.41
1:D:3125:ALA:HB2	1:D:3142:VAL:HG13	2.02	0.41
1:E:4294:ASN:O	1:E:4294:ASN:ND2	2.53	0.41
1:H:7226:PRO:HB3	1:H:7237:ILE:HG21	2.02	0.41
1:A:132:VAL:HG21	3:A:8108:HOH:O	2.20	0.41
1:B:1020:ILE:HG12	1:B:1077:CYS:SG	2.59	0.41
1:B:1042:GLY:O	1:B:1043:PHE:C	2.64	0.41
1:B:1081:LYS:HG3	3:B:8690:HOH:O	2.19	0.41
1:E:4004:ASN:OD1	1:E:4270:LYS:HE2	2.20	0.41
1:E:4133:GLU:OE1	1:E:4136:GLY:HA2	2.20	0.41
1:E:4293:LEU:HD12	1:E:4293:LEU:H	1.86	0.41
1:G:6179:ALA:HA	1:G:6271:ILE:HG13	2.02	0.41
1:C:2205:GLY:HA3	1:D:3145:MET:HE2	2.02	0.41
1:C:2288:LYS:N	3:C:9020:HOH:O	2.52	0.41
1:D:3066:PRO:CG	1:D:3137:ARG:HD2	2.51	0.41
1:D:3097:LEU:HD23	1:D:3097:LEU:C	2.44	0.41
1:G:6224:PHE:O	1:G:6226:PRO:HD3	2.20	0.41
1:A:215:PHE:CE1	1:A:216:LEU:HD13	2.55	0.41
1:C:2221:ASN:HD21	1:C:2223:LYS:HZ3	1.69	0.41
1:C:2281:ASN:C	1:C:2281:ASN:ND2	2.71	0.41
1:F:5002:LYS:HD3	1:F:5007:GLU:HA	2.03	0.41
1:H:7233:GLU:CG	1:H:7234:GLY:N	2.83	0.41
1:A:94:GLN:CG	1:B:1049:MET:HB2	2.50	0.41
1:B:1019:LYS:HB2	1:B:1078:HIS:O	2.21	0.41
1:H:7046:SER:OG	1:H:7048:ILE:HG22	2.21	0.41
1:A:75:GLN:HB2	1:A:194:ILE:HD13	2.02	0.41
1:C:2141:ALA:O	1:C:2143:PRO:HD3	2.21	0.41
1:C:2262:ARG:O	1:C:2266:LEU:HG	2.21	0.41
1:D:3119:PHE:O	1:D:3122:LYS:HG3	2.21	0.41
1:E:4074:ILE:CG2	1:E:4075:GLN:N	2.83	0.41
1:E:4276:LYS:CG	1:E:4277:ILE:N	2.84	0.41
1:F:5060:ALA:HA	1:F:5064:GLU:OE2	2.21	0.41
1:G:6205:GLY:N	1:H:7145:MET:HE2	2.35	0.41
1:H:7008:VAL:HG22	1:H:7277:ILE:HB	2.03	0.41
1:A:46:SER:HB3	1:B:1094:GLN:HE22	1.85	0.41
1:A:185:ASP:OD2	1:D:3029:ASP:HB2	2.21	0.41
1:C:2276:LYS:NZ	1:C:2278:THR:CG2	2.82	0.41
1:H:7173:GLN:NE2	3:H:9655:HOH:O	2.37	0.41
1:E:4214:LYS:C	1:E:4216:LEU:N	2.80	0.40
1:F:5138:LYS:HG2	3:F:8268:HOH:O	2.21	0.40
1:H:7016:PHE:CE1	1:H:7286:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6144:MET:HE3	1:G:6146:GLU:HG2	2.03	0.40
1:C:2029:ASP:HA	1:C:2070:PRO:HG2	2.03	0.40
1:C:2198:PRO:C	1:C:2200:GLY:N	2.79	0.40
1:E:4030:TYR:CZ	1:E:4059:LYS:HD3	2.56	0.40
1:E:4161:ILE:HG22	3:E:8618:HOH:O	2.20	0.40
1:F:5061:LYS:O	1:F:5064:GLU:HG2	2.22	0.40
1:G:6045:THR:CG2	1:G:6198:PRO:HD3	2.51	0.40
1:H:7177:LEU:HD12	3:H:8534:HOH:O	2.21	0.40
1:A:42:GLY:O	1:A:43:PHE:C	2.63	0.40
1:A:202:VAL:HG21	1:A:248:VAL:HG23	2.04	0.40
1:H:7233:GLU:CG	1:H:7234:GLY:H	2.34	0.40
1:B:1012:PHE:CD1	1:B:1290:ILE:HG23	2.56	0.40
1:F:5001:MET:HE1	3:F:9223:HOH:O	2.19	0.40
1:F:5208:VAL:HG23	3:F:8570:HOH:O	2.21	0.40
1:G:6202:VAL:HG21	1:G:6248:VAL:HG23	2.04	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	295/297 (99%)	283 (96%)	8 (3%)	4 (1%)	9	4
1	B	295/297 (99%)	282 (96%)	12 (4%)	1 (0%)	36	35
1	C	295/297 (99%)	282 (96%)	12 (4%)	1 (0%)	36	35
1	D	295/297 (99%)	273 (92%)	18 (6%)	4 (1%)	9	4
1	E	295/297 (99%)	276 (94%)	16 (5%)	3 (1%)	12	8
1	F	295/297 (99%)	284 (96%)	9 (3%)	2 (1%)	18	14
1	G	295/297 (99%)	278 (94%)	15 (5%)	2 (1%)	18	14
1	H	295/297 (99%)	275 (93%)	19 (6%)	1 (0%)	36	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2360/2376 (99%)	2233 (95%)	109 (5%)	18 (1%)	16	11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1208	VAL
1	D	3208	VAL
1	E	4286	LEU
1	F	5208	VAL
1	A	208	VAL
1	A	232	VAL
1	C	2286	LEU
1	D	3110	ASP
1	E	4233	GLU
1	F	5233	GLU
1	D	3111	ALA
1	G	6214	LYS
1	G	6286	LEU
1	E	4210	ALA
1	H	7284	GLY
1	A	233	GLU
1	A	234	GLY
1	D	3209	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/227 (100%)	218 (96%)	9 (4%)	28	27
1	B	227/227 (100%)	218 (96%)	9 (4%)	28	27
1	C	227/227 (100%)	220 (97%)	7 (3%)	35	37
1	D	227/227 (100%)	217 (96%)	10 (4%)	25	24
1	E	227/227 (100%)	222 (98%)	5 (2%)	45	50
1	F	227/227 (100%)	222 (98%)	5 (2%)	45	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	227/227 (100%)	216 (95%)	11 (5%)	23	21
1	H	227/227 (100%)	221 (97%)	6 (3%)	40	44
All	All	1816/1816 (100%)	1754 (97%)	62 (3%)	32	33

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	35	VAL
1	A	97	LEU
1	A	122	LYS
1	A	129	GLN
1	A	216	LEU
1	A	221	ASN
1	A	233	GLU
1	A	297	PHE
1	B	1007	GLU
1	B	1058	ILE
1	B	1069	ARG
1	B	1077	CYS
1	B	1089	LEU
1	B	1104	VAL
1	B	1122	LYS
1	B	1129	GLN
1	B	1144	MET
1	C	2104	VAL
1	C	2120	LYS
1	C	2122	LYS
1	C	2129	GLN
1	C	2191	GLU
1	C	2278	THR
1	C	2281	ASN
1	D	3017	ASP
1	D	3077	CYS
1	D	3104	VAL
1	D	3110	ASP
1	D	3112	GLU
1	D	3129	GLN
1	D	3193	VAL
1	D	3233	GLU
1	D	3271	ILE

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Mol	Chain	Res	Type
1	D	3282	TYR
1	E	4104	VAL
1	E	4115	ASP
1	E	4122	LYS
1	E	4129	GLN
1	E	4217	LYS
1	F	5101	THR
1	F	5104	VAL
1	F	5122	LYS
1	F	5129	GLN
1	F	5253	ASN
1	G	6017	ASP
1	G	6077	CYS
1	G	6104	VAL
1	G	6110	ASP
1	G	6120	LYS
1	G	6129	GLN
1	G	6151	ILE
1	G	6220	THR
1	G	6259	GLU
1	G	6281	ASN
1	G	6285	LYS
1	H	7001	MET
1	H	7104	VAL
1	H	7110	ASP
1	H	7129	GLN
1	H	7153	ASN
1	H	7229	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	38	ASN
1	A	75	GLN
1	A	78	HIS
1	A	94	GLN
1	A	173	GLN
1	A	221	ASN
1	A	281	ASN
1	A	289	HIS
1	B	1004	ASN

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Mol	Chain	Res	Type
1	B	1078	HIS
1	B	1087	GLN
1	B	1094	GLN
1	B	1129	GLN
1	B	1153	ASN
1	B	1221	ASN
1	B	1281	ASN
1	B	1289	HIS
1	C	2004	ASN
1	C	2038	ASN
1	C	2075	GLN
1	C	2078	HIS
1	C	2087	GLN
1	C	2094	GLN
1	C	2129	GLN
1	C	2221	ASN
1	C	2253	ASN
1	C	2281	ASN
1	C	2289	HIS
1	D	3004	ASN
1	D	3038	ASN
1	D	3075	GLN
1	D	3078	HIS
1	D	3087	GLN
1	D	3129	GLN
1	D	3153	ASN
1	D	3173	GLN
1	D	3221	ASN
1	D	3289	HIS
1	D	3292	ASN
1	E	4004	ASN
1	E	4075	GLN
1	E	4078	HIS
1	E	4094	GLN
1	E	4129	GLN
1	E	4153	ASN
1	E	4221	ASN
1	E	4231	GLN
1	E	4281	ASN
1	E	4289	HIS
1	E	4294	ASN
1	F	5004	ASN

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Mol	Chain	Res	Type
1	F	5038	ASN
1	F	5075	GLN
1	F	5078	HIS
1	F	5087	GLN
1	F	5129	GLN
1	F	5153	ASN
1	F	5221	ASN
1	F	5231	GLN
1	F	5253	ASN
1	G	6004	ASN
1	G	6075	GLN
1	G	6078	HIS
1	G	6087	GLN
1	G	6094	GLN
1	G	6129	GLN
1	G	6153	ASN
1	G	6221	ASN
1	G	6281	ASN
1	G	6289	HIS
1	G	6292	ASN
1	H	7075	GLN
1	H	7078	HIS
1	H	7087	GLN
1	H	7129	GLN
1	H	7153	ASN
1	H	7221	ASN
1	H	7253	ASN
1	H	7289	HIS
1	H	7294	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	297/297 (100%)	0.15	9 (3%)	52	51	6, 13, 26, 42	0
1	B	297/297 (100%)	0.24	16 (5%)	31	30	7, 14, 32, 46	0
1	C	297/297 (100%)	0.20	8 (2%)	56	55	7, 14, 28, 41	0
1	D	297/297 (100%)	0.34	24 (8%)	18	17	6, 14, 40, 55	0
1	E	297/297 (100%)	0.41	25 (8%)	17	15	8, 15, 40, 50	0
1	F	297/297 (100%)	0.24	10 (3%)	48	47	6, 15, 29, 40	0
1	G	297/297 (100%)	0.31	13 (4%)	39	38	8, 15, 32, 44	0
1	H	297/297 (100%)	0.27	15 (5%)	33	32	7, 14, 30, 49	0
All	All	2376/2376 (100%)	0.27	120 (5%)	33	32	6, 14, 32, 55	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	7283	GLY	7.7
1	E	4286	LEU	6.0
1	C	2287	GLY	5.9
1	D	3286	LEU	5.8
1	B	1208	VAL	5.2
1	H	7286	LEU	5.2
1	H	7284	GLY	4.9
1	D	3283	GLY	4.7
1	D	3208	VAL	4.7
1	D	3287	GLY	4.7
1	D	3233	GLU	4.5
1	D	3284	GLY	4.3
1	G	6286	LEU	4.2
1	D	3285	LYS	4.0
1	E	4234	GLY	4.0
1	H	7153	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	2115	ASP	3.9
1	E	4287	GLY	3.6
1	G	6287	GLY	3.6
1	E	4232	VAL	3.5
1	H	7285	LYS	3.4
1	E	4233	GLU	3.4
1	D	3240	GLY	3.4
1	D	3209	GLY	3.3
1	D	3016	PHE	3.3
1	D	3282	TYR	3.2
1	E	4288	LYS	3.1
1	G	6284	GLY	3.1
1	B	1233	GLU	3.1
1	F	5287	GLY	3.1
1	D	3232	VAL	3.1
1	F	5208	VAL	3.1
1	A	130	LYS	3.0
1	E	4239	ALA	3.0
1	A	285	LYS	3.0
1	A	232	VAL	3.0
1	B	1285	LYS	3.0
1	E	4285	LYS	2.9
1	H	7112	GLU	2.8
1	A	233	GLU	2.8
1	G	6285	LYS	2.8
1	A	208	VAL	2.8
1	G	6112	GLU	2.7
1	B	1016	PHE	2.7
1	E	4215	PHE	2.7
1	G	6218	ALA	2.7
1	H	7113	GLU	2.7
1	E	4116	ASP	2.7
1	B	1239	ALA	2.7
1	E	4208	VAL	2.7
1	A	286	LEU	2.7
1	B	1294	ASN	2.7
1	G	6151	ILE	2.7
1	B	1286	LEU	2.6
1	E	4231	GLN	2.6
1	E	4294	ASN	2.5
1	E	4235	THR	2.5
1	G	6239	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	3112	GLU	2.5
1	E	4209	GLY	2.5
1	E	4284	GLY	2.5
1	E	4081	LYS	2.5
1	H	7115	ASP	2.5
1	E	4114	LYS	2.5
1	G	6213	TYR	2.5
1	A	287	GLY	2.5
1	G	6294	ASN	2.5
1	D	3113	GLU	2.4
1	F	5112	GLU	2.4
1	H	7234	GLY	2.4
1	B	1290	ILE	2.4
1	D	3132	VAL	2.4
1	H	7288	LYS	2.4
1	C	2239	ALA	2.3
1	H	7114	LYS	2.3
1	E	4213	TYR	2.3
1	B	1113	GLU	2.2
1	G	6016	PHE	2.2
1	G	6215	PHE	2.2
1	A	290	ILE	2.2
1	D	3239	ALA	2.2
1	F	5239	ALA	2.2
1	C	2286	LEU	2.2
1	B	1007	GLU	2.2
1	G	6282	TYR	2.2
1	D	3215	PHE	2.2
1	B	1287	GLY	2.2
1	E	4218	ALA	2.2
1	B	1282	TYR	2.2
1	B	1130	LYS	2.2
1	D	3214	LYS	2.2
1	H	7287	GLY	2.2
1	D	3288	LYS	2.2
1	F	5116	ASP	2.2
1	B	1215	PHE	2.1
1	B	1081	LYS	2.1
1	C	2231	GLN	2.1
1	E	4016	PHE	2.1
1	F	5232	VAL	2.1
1	D	3210	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	7111	ALA	2.1
1	F	5288	LYS	2.1
1	A	234	GLY	2.1
1	B	1232	VAL	2.1
1	C	2114	LYS	2.1
1	E	4138	LYS	2.1
1	C	2112	GLU	2.1
1	H	7233	GLU	2.1
1	H	7294	ASN	2.1
1	D	3213	TYR	2.1
1	E	4282	TYR	2.1
1	E	4113	GLU	2.0
1	C	2288	LYS	2.0
1	D	3217	LYS	2.0
1	F	5138	LYS	2.0
1	F	5209	GLY	2.0
1	F	5132	VAL	2.0
1	D	3111	ALA	2.0
1	E	4229	ARG	2.0
1	D	3234	GLY	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($\text{\AA}^2$)	Q<0.9
2	K	H	8023	1/1	0.95	0.05	17,17,17,17	0
2	K	D	8012	1/1	0.97	0.04	12,12,12,12	0
2	K	F	8010	1/1	0.97	0.04	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	K	G	8021	1/1	0.97	0.04	15,15,15,15	0
2	K	H	8004	1/1	0.97	0.05	11,11,11,11	0
2	K	A	8011	1/1	0.97	0.03	11,11,11,11	0
2	K	F	8009	1/1	0.98	0.03	11,11,11,11	0
2	K	C	8014	1/1	0.98	0.03	15,15,15,15	0
2	K	B	8015	1/1	0.98	0.02	13,13,13,13	0
2	K	E	8016	1/1	0.98	0.04	17,17,17,17	0
2	K	E	8024	1/1	0.98	0.03	16,16,16,16	0
2	K	B	8017	1/1	0.99	0.03	11,11,11,11	0
2	K	E	8018	1/1	0.99	0.03	12,12,12,12	0
2	K	C	8001	1/1	0.99	0.02	11,11,11,11	0
2	K	C	8007	1/1	0.99	0.03	11,11,11,11	0
2	K	B	8005	1/1	0.99	0.03	11,11,11,11	0
2	K	G	8008	1/1	0.99	0.02	10,10,10,10	0
2	K	G	8013	1/1	0.99	0.04	12,12,12,12	0
2	K	D	8003	1/1	0.99	0.02	10,10,10,10	0
2	K	D	8006	1/1	0.99	0.04	9,9,9,9	0
2	K	H	8020	1/1	0.99	0.03	14,14,14,14	0
2	K	A	8002	1/1	0.99	0.02	10,10,10,10	0
2	K	A	8019	1/1	1.00	0.04	14,14,14,14	0
2	K	F	8022	1/1	1.00	0.03	14,14,14,14	0

6.5 Other polymers

There are no such residues in this entry.