



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:35 PM UTC

PDB ID : 1PZN / pdb_00001pzn
Title : Rad51 (RadA)
Authors : Shin, D.S.; Tainer, J.A.
Deposited on : 2003-07-12
Resolution : 2.85 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

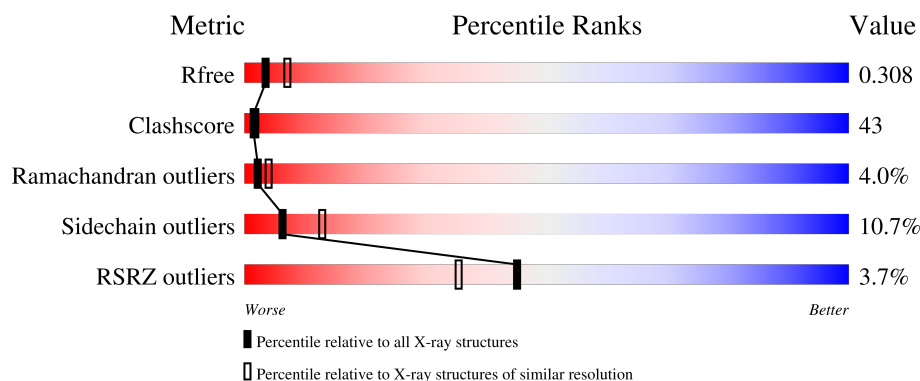
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	349	38% 38% 9% 14%
1	B	349	28% 33% 8% 32%
1	C	349	29% 31% 7% 32%
1	D	349	26% 33% 9% 32%
1	E	349	32% 29% 7% 32%

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Mol	Chain	Length	Quality of chain
1	F	349	
1	G	349	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IMD	B	359	-	-	X	-
4	GOL	A	374	-	X	-	-
4	GOL	B	367	-	X	-	-
4	GOL	C	368	-	X	-	-
4	GOL	C	370	-	X	-	-
4	GOL	D	369	-	X	-	-
4	GOL	E	371	-	X	-	-
4	GOL	F	366	-	X	-	-
4	GOL	F	372	-	X	-	-
4	GOL	F	373	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13820 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 DNA repair and recombination protein rad51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	Se	0	0	0
			2317	1458	419	437	3			
1	B	239	Total	C	N	O	Se	0	0	0
			1879	1184	343	349	3			
1	C	239	Total	C	N	O	Se	0	0	0
			1879	1184	343	349	3			
1	D	239	Total	C	N	O	Se	0	0	0
			1879	1184	343	349	3			
1	E	239	Total	C	N	O	Se	0	0	0
			1879	1184	343	349	3			
1	F	239	Total	C	N	O	Se	0	0	0
			1879	1184	343	349	3			
1	G	238	Total	C	N	O	Se	0	0	0
			1875	1182	342	348	3			

There are 28 discrepancies between the modelled and reference sequences:

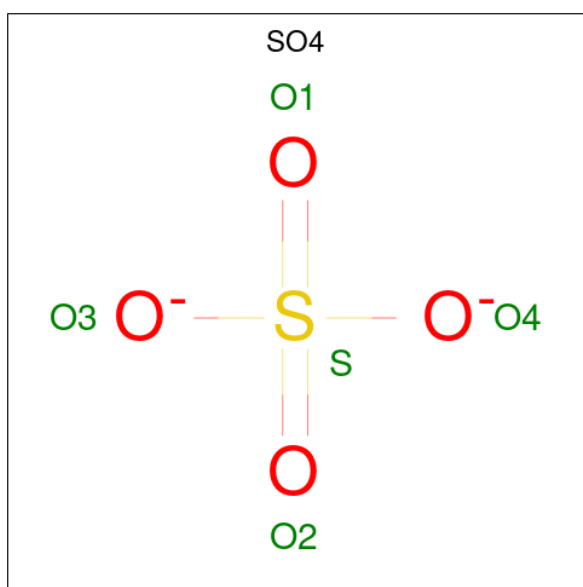
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP O74036
A	98	MSE	MET	modified residue	UNP O74036
A	154	MSE	MET	modified residue	UNP O74036
A	212	MSE	MET	modified residue	UNP O74036
B	1	MSE	MET	modified residue	UNP O74036
B	98	MSE	MET	modified residue	UNP O74036
B	154	MSE	MET	modified residue	UNP O74036
B	212	MSE	MET	modified residue	UNP O74036
C	1	MSE	MET	modified residue	UNP O74036
C	98	MSE	MET	modified residue	UNP O74036
C	154	MSE	MET	modified residue	UNP O74036
C	212	MSE	MET	modified residue	UNP O74036
D	1	MSE	MET	modified residue	UNP O74036
D	98	MSE	MET	modified residue	UNP O74036
D	154	MSE	MET	modified residue	UNP O74036

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Chain	Residue	Modelled	Actual	Comment	Reference
D	212	MSE	MET	modified residue	UNP O74036
E	1	MSE	MET	modified residue	UNP O74036
E	98	MSE	MET	modified residue	UNP O74036
E	154	MSE	MET	modified residue	UNP O74036
E	212	MSE	MET	modified residue	UNP O74036
F	1	MSE	MET	modified residue	UNP O74036
F	98	MSE	MET	modified residue	UNP O74036
F	154	MSE	MET	modified residue	UNP O74036
F	212	MSE	MET	modified residue	UNP O74036
G	1	MSE	MET	modified residue	UNP O74036
G	98	MSE	MET	modified residue	UNP O74036
G	154	MSE	MET	modified residue	UNP O74036
G	212	MSE	MET	modified residue	UNP O74036

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



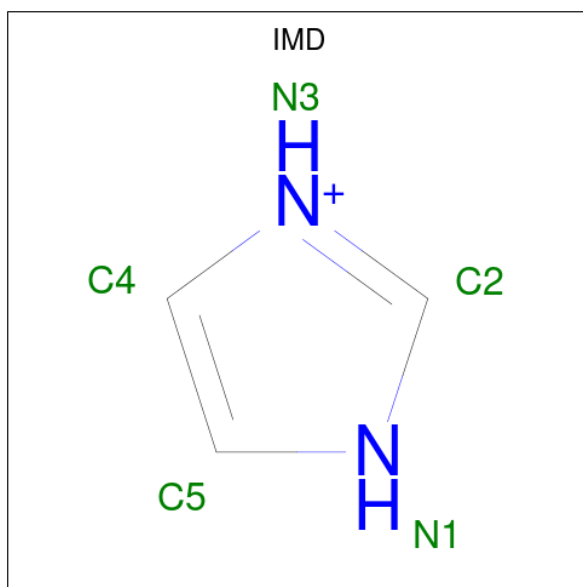
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	A	1	Total	C	N	0	0
			5	3	2		
3	A	1	Total	C	N	0	0
			5	3	2		
3	A	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	C	1	Total	C	N	0	0
			5	3	2		
3	F	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		
5	E	1	Total	C	O	0	0
			8	6	2		
5	G	1	Total	C	O	0	0
			8	6	2		
5	G	1	Total	C	O	0	0
			8	6	2		

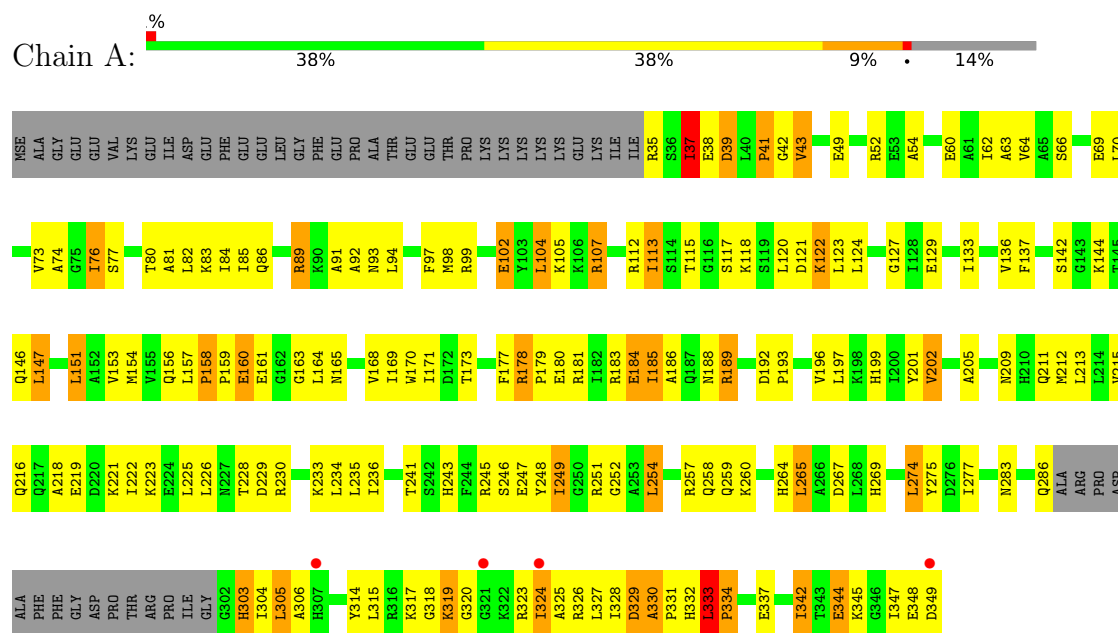
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	6	Total	O	0	0
			6	6		
6	C	7	Total	O	0	0
			7	7		
6	D	11	Total	O	0	0
			11	11		
6	E	10	Total	O	0	0
			10	10		
6	F	6	Total	O	0	0
			6	6		
6	G	7	Total	O	0	0
			7	7		

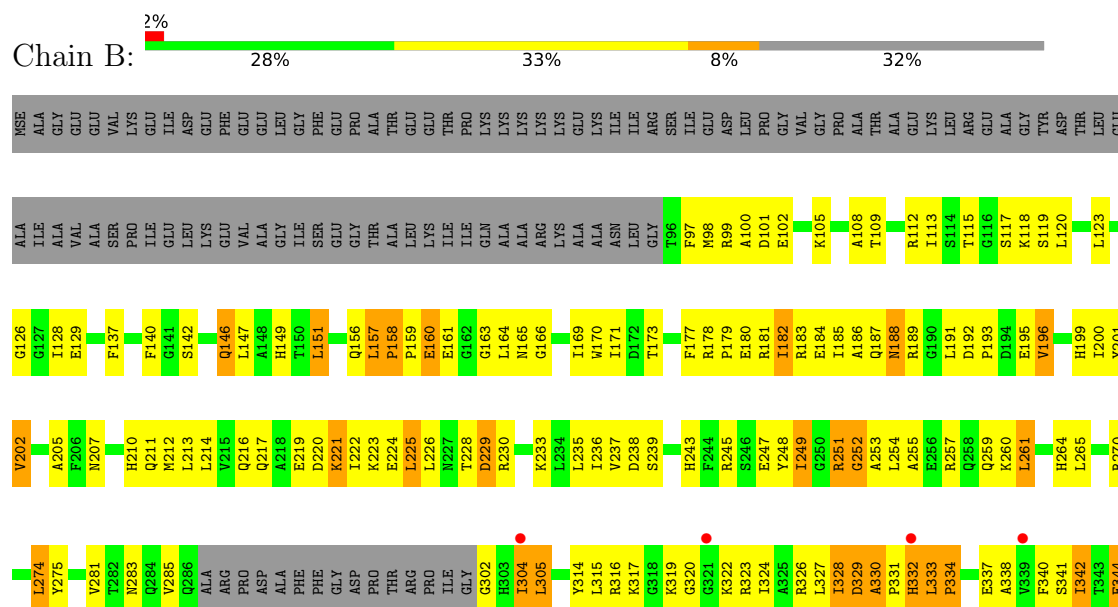
3 Residue-property plots

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: DNA repair and recombination protein rad51



- Molecule 1: DNA repair and recombination protein rad51



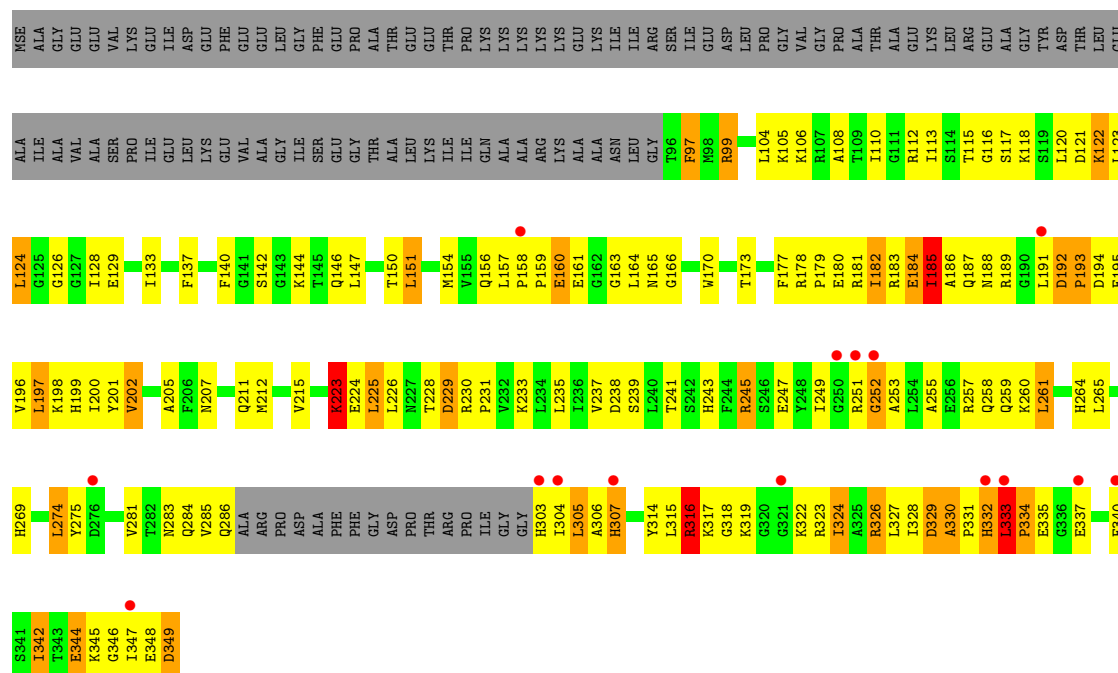
[illegible]

Chain F:

4% 28% 34% 5% 32%

MSE
ALA
ILE
GLY
GLU
VAL
SER
PRO
ILE
GLU
ASP
LEU
LYS
PHE
GLU
PHE
GLU
LEU
GLY
VAL
ALA
GLY
ILE
SER
GLY
GLY
THR
ALA
GLU
LYS
GLU
THR
ILE
GLN
ALA
ALA
LYS
ARG
GLY
T96
F97
M98
R99
A100
D101
E102
Y103
L104
K105
K106
R107
A108
T109
I113
S114
T115
G116
S117
K118
K122
Y123
E129
F137
F140
G141
G142
G143
K144
T145
Q146
L147
L151
Q156
L157
P158
P159
E160
E161
G162
L164
M165
G166
T169
W170
I171
D172
E174
N175
T176
T177
T178
M179
E180
R181
I182
E183
E184
I185
M188
R189
G190
L191
D192
P193
D194
E195
V196
L197
K198
H199
I200
Y201
W202
A203
R204
F206
N207
Q211
M212
L213
L214
V215
Q216
Q217
A218
E219
D220
K221
L222
K223
L226
N227
T228
D229
R230
P231
V232
K233
L234
L235
I236
V237
D238
S239
L240
T241
S242
H243
F244
R245
G246
E247
G250
R251
G252
A253
L254
A255
Q258
Q259
K260
L261
H264
L265
H269
P270
L274
Y275
V281
N283
Q284
V285
Q286
A287
ARG
PRO
ASP
ALA
PHE
PHE
GLY
ASP
PRO
THR
ARG
PRO
ILE
GLY
G302
H303
L304
L305
A306
H307
S308
Y314
L315
R316
K317
G318
K319
G320
G321
K322
R323
I324
A325
R326
L327
I328
D329
A330
P331
H332
L333
P334
E335
G336
E337
A338
V339
F340
S341
I342
T343
E344
K345
G346
I347
E348
D349

Chain G: 4% 27% 32% 8% 32%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	144.16Å 193.12Å 176.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.12 – 2.85 39.12 – 2.85	Depositor EDS
% Data completeness (in resolution range)	95.3 (39.12-2.85) 97.3 (39.12-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.307 0.263 , 0.308	Depositor DCC
R_{free} test set	5206 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13820	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: GOL, SO4, MPD, IMD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	0/2347	1.07	11/3159 (0.3%)
1	B	0.55	0/1905	1.01	7/2560 (0.3%)
1	C	0.50	0/1905	1.08	15/2560 (0.6%)
1	D	0.49	0/1905	1.03	13/2560 (0.5%)
1	E	0.61	0/1905	1.06	9/2560 (0.4%)
1	F	0.54	0/1905	1.03	4/2560 (0.2%)
1	G	0.53	1/1901 (0.1%)	1.06	16/2555 (0.6%)
All	All	0.55	1/13773 (0.0%)	1.05	75/18514 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	128	ILE	CA-CB	6.72	1.61	1.54

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	344	GLU	N-CA-C	-10.62	96.51	110.53
1	G	344	GLU	N-CA-C	-10.60	96.54	110.53
1	F	344	GLU	N-CA-C	-10.08	97.23	110.53
1	B	344	GLU	N-CA-C	-10.04	97.28	110.53
1	A	344	GLU	N-CA-C	-9.92	97.43	110.53
1	C	344	GLU	N-CA-C	-9.91	97.44	110.53
1	D	344	GLU	N-CA-C	-9.83	97.55	110.53
1	A	39	ASP	N-CA-C	-9.01	100.37	112.26
1	C	333	LEU	CA-C-N	8.04	129.89	119.84
1	C	333	LEU	C-N-CA	8.04	129.89	119.84
1	F	182	ILE	N-CA-C	-8.00	102.90	110.42
1	A	122	LYS	N-CA-C	-7.88	102.64	111.07
1	G	252	GLY	N-CA-C	-7.24	105.50	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	VAL	N-CA-C	7.07	118.31	107.99
1	C	252	GLY	N-CA-C	-6.74	104.03	115.08
1	C	158	PRO	CA-C-N	6.71	126.22	119.24
1	C	158	PRO	C-N-CA	6.71	126.22	119.24
1	C	257	ARG	N-CA-C	-6.67	103.94	111.14
1	E	157	LEU	CA-C-N	6.65	124.52	119.66
1	E	157	LEU	C-N-CA	6.65	124.52	119.66
1	B	157	LEU	CA-C-N	6.58	124.46	119.66
1	B	157	LEU	C-N-CA	6.58	124.46	119.66
1	G	333	LEU	CA-C-N	6.43	127.88	119.84
1	G	333	LEU	C-N-CA	6.43	127.88	119.84
1	D	189	ARG	N-CA-C	-6.35	103.20	111.71
1	D	204	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	G	245	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	E	103	TYR	N-CA-C	-6.10	103.96	111.40
1	E	158	PRO	N-CA-C	6.01	116.24	110.47
1	B	158	PRO	N-CA-C	6.00	116.23	110.47
1	D	158	PRO	CA-C-N	5.99	126.14	119.32
1	D	158	PRO	C-N-CA	5.99	126.14	119.32
1	G	182	ILE	N-CA-C	-5.88	104.90	110.42
1	F	204	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	C	157	LEU	CA-C-N	5.86	123.94	119.66
1	C	157	LEU	C-N-CA	5.86	123.94	119.66
1	A	158	PRO	CA-C-N	5.83	125.31	119.24
1	A	158	PRO	C-N-CA	5.83	125.31	119.24
1	G	253	ALA	N-CA-C	-5.80	106.85	114.04
1	A	178	ARG	NE-CZ-NH2	-5.79	113.99	119.20
1	F	204	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	C	307	HIS	N-CA-C	5.74	117.62	111.36
1	D	204	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	G	319	LYS	CB-CA-C	-5.68	110.00	116.54
1	C	253	ALA	N-CA-C	-5.64	98.78	110.80
1	C	103	TYR	N-CA-C	-5.58	105.35	111.82
1	B	158	PRO	CA-C-N	5.55	125.02	119.24
1	B	158	PRO	C-N-CA	5.55	125.02	119.24
1	D	146	GLN	N-CA-C	-5.55	105.15	111.14
1	A	333	LEU	CA-C-N	5.53	126.75	119.84
1	A	333	LEU	C-N-CA	5.53	126.75	119.84
1	E	252	GLY	N-CA-C	-5.53	106.39	114.90
1	G	316	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	B	146	GLN	N-CA-C	-5.49	105.21	111.14
1	D	198	LYS	N-CA-C	-5.49	105.94	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	328	ILE	N-CA-C	5.48	114.70	106.42
1	G	226	LEU	N-CA-C	-5.41	105.54	111.82
1	A	189	ARG	N-CA-C	-5.40	104.95	112.30
1	D	116	GLY	N-CA-C	-5.35	107.83	115.64
1	G	245	ARG	NE-CZ-NH1	5.29	126.80	121.50
1	D	316	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	C	146	GLN	N-CA-C	-5.27	105.45	111.14
1	C	219	GLU	N-CA-C	-5.26	105.63	111.36
1	C	316	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	D	185	ILE	N-CA-C	-5.23	107.49	111.62
1	E	104	LEU	N-CA-C	-5.21	105.08	111.75
1	G	245	ARG	CD-NE-CZ	5.21	131.70	124.40
1	D	310	THR	N-CA-C	-5.14	107.67	114.04
1	D	316	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	G	192	ASP	CA-C-N	5.11	126.23	119.84
1	G	192	ASP	C-N-CA	5.11	126.23	119.84
1	G	316	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	A	226	LEU	N-CA-C	-5.02	103.91	110.53
1	E	187	GLN	N-CA-C	-5.02	107.22	113.19
1	G	245	ARG	CG-CD-NE	-5.00	101.00	112.00

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	2317	0	2375	218	0
1	B	1879	0	1917	198	0
1	C	1879	0	1917	164	0
1	D	1879	0	1917	191	0
1	E	1879	0	1917	143	0
1	F	1879	0	1917	169	0
1	G	1875	0	1914	181	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	1	0
2	G	5	0	0	1	0
3	A	20	0	20	2	0
3	B	15	0	15	8	0
3	C	5	0	5	0	0
3	F	5	0	5	2	0
4	A	6	0	5	0	0
4	B	6	0	4	1	0
4	C	12	0	9	1	0
4	D	6	0	4	2	0
4	E	6	0	4	0	0
4	F	18	0	13	2	0
5	B	8	0	14	0	0
5	E	8	0	14	0	0
5	G	16	0	28	0	0
6	A	20	0	0	5	0
6	B	6	0	0	2	0
6	C	7	0	0	6	0
6	D	11	0	0	2	0
6	E	10	0	0	0	0
6	F	6	0	0	1	0
6	G	7	0	0	0	0
All	All	13820	0	14014	1193	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 43.

All (1193) 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)
4:D:369:GOL:C1	4:D:369:GOL:O1	1.64	1.46
4:F:373:GOL:C1	4:F:373:GOL:O1	1.65	1.42
1:F:324:ILE:HD11	1:F:337:GLU:HB3	1.28	1.11
1:A:317:LYS:HG3	1:A:323:ARG:HH12	0.98	1.10
1:B:324:ILE:HD11	1:B:337:GLU:HB3	1.34	1.09
1:E:330:ALA:H	1:E:331:PRO:HD2	1.15	1.06
1:B:228:THR:HG22	1:B:230:ARG:H	1.18	1.05
1:A:107:ARG:HH11	1:A:107:ARG:HB3	1.16	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:HG3	1:A:323:ARG:NH1	1.73	1.04
1:B:329:ASP:HB3	1:B:331:PRO:HD2	1.41	1.02
1:D:169:ILE:HG13	1:D:222:ILE:HD11	1.44	1.00
1:D:222:ILE:HD12	1:D:232:VAL:HG21	1.42	0.99
1:F:258:GLN:HE21	1:F:258:GLN:HA	1.27	0.98
1:D:183:ARG:HD2	1:D:193:PRO:HB2	1.45	0.97
1:E:156:GLN:NE2	1:E:196:VAL:HG13	1.79	0.97
1:A:330:ALA:H	1:A:331:PRO:HD2	1.30	0.96
1:C:251:ARG:HB3	1:D:251:ARG:HB2	1.48	0.96
1:G:317:LYS:HG3	1:G:323:ARG:HH12	1.29	0.96
1:D:187:GLN:HB3	1:D:193:PRO:HD3	1.44	0.96
1:C:107:ARG:HB3	1:C:107:ARG:HH11	1.30	0.95
1:A:246:SER:O	1:A:249:ILE:HD11	1.70	0.91
1:G:189:ARG:HH21	1:G:345:LYS:HB3	1.34	0.90
1:F:286:GLN:H	1:F:286:GLN:NE2	1.70	0.88
1:D:326:ARG:HH21	1:D:326:ARG:HB3	1.36	0.88
1:B:212:MSE:HE1	1:B:260:LYS:HD3	1.56	0.88
1:C:107:ARG:HB3	1:C:107:ARG:NH1	1.88	0.88
1:G:187:GLN:HB3	1:G:193:PRO:HB3	1.55	0.88
1:A:326:ARG:HD3	1:A:337:GLU:HG2	1.55	0.88
1:C:212:MSE:HE1	1:C:260:LYS:HD2	1.57	0.87
1:D:330:ALA:H	1:D:331:PRO:HD2	1.39	0.87
1:E:327:LEU:HD21	1:E:333:LEU:HD23	1.55	0.87
1:E:269:HIS:NE2	1:E:308:SER:HB3	1.89	0.86
1:E:157:LEU:HD13	1:E:161:GLU:HB2	1.57	0.86
1:A:249:ILE:HD12	1:A:249:ILE:N	1.90	0.86
1:B:330:ALA:H	1:B:331:PRO:HD2	1.37	0.86
1:A:157:LEU:HD13	1:A:161:GLU:CB	2.06	0.85
1:B:169:ILE:HD11	1:B:221:LYS:HG2	1.58	0.85
1:A:317:LYS:CG	1:A:323:ARG:HH12	1.86	0.85
1:D:317:LYS:HG3	1:D:323:ARG:HH12	1.42	0.85
1:C:330:ALA:H	1:C:331:PRO:HD2	1.40	0.85
1:A:37:ILE:HD11	1:A:52:ARG:HH12	1.42	0.85
1:G:115:THR:HG21	1:G:120:LEU:HD22	1.56	0.84
1:C:251:ARG:NH2	1:D:251:ARG:HA	1.93	0.83
1:D:261:LEU:HD22	1:D:304:ILE:HD11	1.60	0.83
1:C:185:ILE:HD12	1:C:346:GLY:N	1.94	0.83
1:F:228:THR:HG22	1:F:229:ASP:H	1.43	0.83
1:D:189:ARG:HH21	1:D:345:LYS:HB3	1.43	0.83
1:C:181:ARG:NH2	1:C:185:ILE:HD11	1.94	0.83
1:E:96:THR:HG22	1:E:97:PHE:H	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:332:HIS:O	1:G:333:LEU:HB2	1.76	0.83
1:F:340:PHE:HA	1:F:349:ASP:HB2	1.61	0.82
1:G:154:MSE:SE	1:G:189:ARG:HH11	2.11	0.82
1:F:228:THR:HG22	1:F:229:ASP:N	1.95	0.82
1:B:252:GLY:CA	3:B:359:IMD:HN3	1.92	0.82
1:A:252:GLY:H	1:G:251:ARG:NH2	1.77	0.82
1:G:181:ARG:O	1:G:185:ILE:HG22	1.80	0.81
1:F:245:ARG:HB3	1:F:304:ILE:HD11	1.62	0.81
1:A:212:MSE:HE1	1:A:260:LYS:HD3	1.61	0.81
1:B:304:ILE:HD13	1:B:305:LEU:N	1.94	0.81
1:A:252:GLY:H	1:G:251:ARG:HH22	1.28	0.81
1:C:157:LEU:HD13	1:C:161:GLU:HB2	1.63	0.81
1:C:251:ARG:HH21	1:D:251:ARG:HA	1.45	0.81
1:B:317:LYS:HG3	1:B:323:ARG:HH22	1.46	0.80
1:F:219:GLU:OE1	1:F:270:ARG:NH2	2.14	0.80
1:F:324:ILE:HD13	1:F:325:ALA:N	1.96	0.80
1:G:348:GLU:O	1:G:349:ASP:HB2	1.82	0.80
1:B:328:ILE:N	1:B:328:ILE:HD12	1.97	0.79
1:A:144:LYS:HG2	2:A:350:SO4:O1	1.82	0.79
1:F:258:GLN:HA	1:F:258:GLN:NE2	1.98	0.79
1:E:330:ALA:H	1:E:331:PRO:CD	1.93	0.78
1:A:80:THR:HA	1:A:83:LYS:HE2	1.63	0.78
1:D:285:VAL:O	1:D:286:GLN:HB3	1.82	0.78
1:C:173:THR:HG22	1:C:205:ALA:HB3	1.66	0.78
1:C:329:ASP:HB2	1:C:331:PRO:HD2	1.65	0.78
1:D:114:SER:HA	1:D:121:ASP:OD2	1.83	0.78
1:A:330:ALA:N	1:A:331:PRO:HD2	1.98	0.78
1:D:188:ASN:OD1	1:D:344:GLU:HB3	1.84	0.78
1:B:330:ALA:H	1:B:331:PRO:CD	1.98	0.77
1:A:107:ARG:HB3	1:A:107:ARG:NH1	1.98	0.77
1:D:332:HIS:CE1	1:E:178:ARG:HE	2.03	0.77
1:E:286:GLN:H	1:E:303:HIS:CE1	2.03	0.77
1:A:107:ARG:HH11	1:A:107:ARG:CB	1.96	0.77
1:A:157:LEU:HD13	1:A:161:GLU:HB3	1.67	0.77
1:G:163:GLY:O	1:G:164:LEU:HD22	1.85	0.76
1:A:160:GLU:CD	1:A:160:GLU:H	1.91	0.76
1:F:173:THR:HG22	1:F:205:ALA:HB3	1.66	0.76
1:D:139:GLU:OE1	1:D:286:GLN:HG2	1.86	0.76
1:C:104:LEU:HD22	1:C:104:LEU:O	1.84	0.76
1:A:74:ALA:HB3	1:A:76:ILE:HD12	1.67	0.75
1:B:314:TYR:CB	1:B:328:ILE:HD11	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:GLN:HE21	1:C:193:PRO:HG3	1.49	0.75
1:A:38:GLU:HB2	6:A:430:HOH:O	1.86	0.75
1:A:221:LYS:HG3	1:A:225:LEU:HD13	1.68	0.75
1:B:252:GLY:HA2	3:B:359:IMD:HN3	1.50	0.75
1:B:146:GLN:HA	1:B:146:GLN:HE21	1.52	0.75
1:D:332:HIS:C	1:D:333:LEU:HD22	2.12	0.75
1:G:117:SER:HB3	1:G:347:ILE:HG22	1.69	0.75
1:A:332:HIS:O	1:A:333:LEU:HB2	1.85	0.75
1:A:324:ILE:CD1	1:A:337:GLU:HB3	2.17	0.74
1:D:156:GLN:NE2	1:D:196:VAL:HG12	2.02	0.74
1:G:113:ILE:HD13	1:G:164:LEU:HD23	1.70	0.74
1:G:317:LYS:HG3	1:G:323:ARG:NH1	2.02	0.74
1:G:324:ILE:HD13	1:G:324:ILE:C	2.12	0.74
1:C:99:ARG:HG2	1:C:101:ASP:OD2	1.87	0.74
1:A:199:HIS:HA	6:A:437:HOH:O	1.87	0.74
1:E:261:LEU:HG	1:E:304:ILE:HD11	1.69	0.73
1:G:225:LEU:HD11	1:G:230:ARG:O	1.86	0.73
1:D:186:ALA:HB1	1:D:196:VAL:HG21	1.70	0.73
1:D:311:LEU:HD11	1:D:327:LEU:HD22	1.71	0.73
1:F:241:THR:HB	1:F:304:ILE:HD12	1.70	0.73
1:E:173:THR:HG22	1:E:205:ALA:HB3	1.71	0.73
1:C:170:TRP:HB3	1:C:202:VAL:HG12	1.71	0.73
1:A:37:ILE:CG1	1:A:38:GLU:H	2.02	0.73
1:B:163:GLY:O	1:B:164:LEU:HD23	1.89	0.73
1:B:157:LEU:HD13	1:B:161:GLU:CB	2.19	0.72
1:G:157:LEU:HD13	1:G:161:GLU:HB2	1.71	0.72
1:E:304:ILE:HG12	1:E:305:LEU:N	2.03	0.72
1:G:185:ILE:HA	1:G:345:LYS:H	1.52	0.72
1:C:194:ASP:O	1:C:198:LYS:HE3	1.88	0.72
1:B:328:ILE:HD12	1:B:328:ILE:H	1.53	0.72
1:C:187:GLN:HB3	1:C:193:PRO:HD3	1.72	0.72
1:G:187:GLN:HB3	1:G:193:PRO:CB	2.18	0.72
1:A:344:GLU:H	1:A:344:GLU:CD	1.98	0.72
1:C:146:GLN:HA	1:C:146:GLN:HE21	1.53	0.72
1:G:156:GLN:NE2	1:G:196:VAL:HG13	2.04	0.72
1:D:157:LEU:HD13	1:D:161:GLU:HB2	1.70	0.71
1:D:182:ILE:HD13	1:D:200:ILE:HD12	1.71	0.71
1:C:163:GLY:O	1:C:164:LEU:HD23	1.90	0.71
1:G:118:LYS:HB2	1:G:349:ASP:O	1.89	0.71
1:A:252:GLY:N	1:G:251:ARG:HH22	1.87	0.71
1:A:330:ALA:H	1:A:331:PRO:CD	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLN:NE2	1:C:196:VAL:HG13	2.04	0.71
1:E:146:GLN:HE21	1:E:146:GLN:HA	1.55	0.71
1:E:327:LEU:C	1:E:328:ILE:HD12	2.15	0.71
1:G:316:ARG:NH1	1:G:324:ILE:HD12	2.06	0.71
1:E:261:LEU:HD13	1:E:261:LEU:C	2.15	0.71
1:B:123:LEU:HD12	1:B:334:PRO:HG2	1.71	0.70
1:B:158:PRO:HD2	1:B:161:GLU:HG3	1.73	0.70
1:F:103:TYR:O	1:F:107:ARG:HG3	1.92	0.70
1:B:323:ARG:HE	1:B:342:ILE:HG13	1.57	0.70
1:F:304:ILE:HG22	1:F:305:LEU:H	1.56	0.70
1:C:181:ARG:HH22	1:C:185:ILE:HD11	1.55	0.70
1:B:118:LYS:H	1:B:349:ASP:HB2	1.54	0.70
1:A:63:ALA:O	1:A:89:ARG:HD3	1.91	0.70
1:F:146:GLN:HE21	1:F:146:GLN:HA	1.56	0.70
1:A:328:ILE:HG22	1:A:328:ILE:O	1.91	0.70
1:C:170:TRP:HB3	1:C:202:VAL:CG1	2.22	0.70
1:C:330:ALA:N	1:C:331:PRO:HD2	2.06	0.70
1:C:331:PRO:O	1:C:332:HIS:HB2	1.90	0.70
1:D:115:THR:HG21	1:D:120:LEU:HD12	1.72	0.70
1:D:160:GLU:CD	1:D:160:GLU:H	1.99	0.69
1:G:185:ILE:HG13	1:G:345:LYS:HA	1.72	0.69
1:A:156:GLN:NE2	1:A:196:VAL:HG13	2.07	0.69
1:B:170:TRP:HB3	1:B:202:VAL:HG12	1.73	0.69
1:G:187:GLN:HE21	1:G:193:PRO:HG3	1.58	0.69
1:D:146:GLN:HE21	1:D:146:GLN:HA	1.57	0.69
1:E:230:ARG:HB3	1:E:230:ARG:NH1	2.08	0.69
1:G:344:GLU:CD	1:G:344:GLU:H	1.99	0.69
1:A:251:ARG:HE	1:B:251:ARG:NH2	1.91	0.69
1:A:258:GLN:HG3	1:B:249:ILE:CD1	2.22	0.69
1:E:157:LEU:HD13	1:E:161:GLU:CB	2.23	0.69
1:B:219:GLU:CD	1:B:270:ARG:HH22	2.01	0.69
1:E:177:PHE:CD2	1:E:202:VAL:HG11	2.28	0.69
1:E:328:ILE:O	1:E:329:ASP:HB3	1.91	0.69
1:G:185:ILE:HG13	1:G:345:LYS:CA	2.23	0.69
1:F:221:LYS:NZ	3:F:363:IMD:H4	2.07	0.69
1:B:324:ILE:HD11	1:B:337:GLU:CB	2.18	0.68
1:B:333:LEU:HB3	1:B:334:PRO:HD2	1.75	0.68
1:B:344:GLU:CD	1:B:344:GLU:H	2.01	0.68
1:G:146:GLN:HE21	1:G:146:GLN:HA	1.57	0.68
1:D:317:LYS:HG3	1:D:323:ARG:NH1	2.07	0.68
1:E:221:LYS:HE3	1:E:225:LEU:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:LEU:HD12	1:E:275:TYR:CZ	2.29	0.68
1:B:157:LEU:HD13	1:B:161:GLU:HB2	1.75	0.68
1:C:187:GLN:NE2	1:C:193:PRO:HG3	2.09	0.68
1:E:124:LEU:HA	1:E:333:LEU:HD21	1.75	0.68
1:A:249:ILE:HD13	1:G:258:GLN:HG3	1.75	0.68
1:D:330:ALA:N	1:D:331:PRO:HD2	2.08	0.68
1:D:327:LEU:C	1:D:328:ILE:HD12	2.19	0.68
1:D:159:PRO:HD3	1:D:165:ASN:ND2	2.09	0.68
1:C:344:GLU:H	1:C:344:GLU:CD	2.02	0.68
1:F:142:SER:O	1:F:323:ARG:HD2	1.94	0.68
1:G:189:ARG:NH2	1:G:345:LYS:HB3	2.08	0.68
1:B:213:LEU:HG	1:B:217:GLN:OE1	1.94	0.67
1:B:317:LYS:HG3	1:B:323:ARG:NH2	2.08	0.67
1:C:159:PRO:HD3	1:C:165:ASN:ND2	2.08	0.67
1:C:304:ILE:HG12	1:C:305:LEU:N	2.09	0.67
1:D:173:THR:HG22	1:D:205:ALA:HB3	1.75	0.67
1:B:146:GLN:HE22	1:B:181:ARG:HE	1.42	0.67
1:F:326:ARG:HD3	1:F:337:GLU:HG2	1.76	0.67
1:F:113:ILE:HD11	1:F:164:LEU:HD12	1.75	0.67
1:B:173:THR:HG22	1:B:205:ALA:HB3	1.77	0.67
1:F:228:THR:CG2	1:F:229:ASP:H	2.06	0.67
1:F:344:GLU:H	1:F:344:GLU:CD	2.03	0.67
1:C:107:ARG:HH11	1:C:107:ARG:CB	2.06	0.67
1:C:188:ASN:ND2	1:C:188:ASN:O	2.26	0.67
1:C:181:ARG:HH22	1:C:185:ILE:CD1	2.08	0.67
1:E:96:THR:HG22	1:E:97:PHE:N	2.10	0.67
1:G:229:ASP:OD2	1:G:229:ASP:N	2.28	0.67
1:C:225:LEU:HB3	1:C:231:PRO:HA	1.76	0.66
1:A:74:ALA:HB3	1:A:76:ILE:CD1	2.25	0.66
1:A:324:ILE:HD11	1:A:337:GLU:HB3	1.76	0.66
1:G:182:ILE:HB	1:G:197:LEU:HD21	1.76	0.66
1:C:177:PHE:CD2	1:C:202:VAL:HG11	2.31	0.66
1:D:329:ASP:CG	1:D:330:ALA:H	2.02	0.66
1:E:189:ARG:HE	1:E:345:LYS:HB3	1.61	0.66
1:E:328:ILE:O	1:E:328:ILE:HG22	1.95	0.66
1:B:330:ALA:N	1:B:331:PRO:CD	2.59	0.66
1:G:159:PRO:HD3	1:G:165:ASN:ND2	2.10	0.66
1:D:327:LEU:HD13	1:D:333:LEU:HB3	1.78	0.66
1:G:154:MSE:SE	1:G:189:ARG:NH1	2.79	0.65
1:D:177:PHE:CD2	1:D:202:VAL:HG11	2.30	0.65
1:D:344:GLU:CD	1:D:344:GLU:H	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:LEU:HD12	1:F:275:TYR:CZ	2.31	0.65
1:D:222:ILE:HG21	1:D:277:ILE:HD11	1.78	0.65
1:F:189:ARG:HH21	1:F:189:ARG:HG3	1.61	0.65
1:G:177:PHE:CD2	1:G:202:VAL:HG11	2.32	0.65
1:F:213:LEU:O	1:F:217:GLN:HG3	1.96	0.65
1:B:192:ASP:OD2	1:B:195:GLU:HB2	1.96	0.65
1:F:327:LEU:O	1:F:328:ILE:HD13	1.97	0.65
1:B:274:LEU:HD12	1:B:275:TYR:CZ	2.32	0.65
1:D:328:ILE:O	1:D:328:ILE:HG22	1.96	0.65
1:F:171:ILE:HG23	1:F:214:LEU:HD23	1.77	0.65
1:D:189:ARG:HB3	1:D:345:LYS:HG2	1.77	0.65
1:G:170:TRP:HB3	1:G:202:VAL:HG12	1.79	0.65
1:E:344:GLU:CD	1:E:344:GLU:H	2.05	0.64
1:B:170:TRP:HB3	1:B:202:VAL:CG1	2.27	0.64
1:C:225:LEU:H	1:C:225:LEU:HD22	1.62	0.64
1:D:189:ARG:HE	1:D:345:LYS:HB3	1.63	0.64
1:A:37:ILE:CD1	1:A:38:GLU:H	2.11	0.64
1:C:251:ARG:CB	1:D:251:ARG:HB2	2.25	0.64
1:F:156:GLN:NE2	1:F:196:VAL:HG13	2.13	0.64
1:A:178:ARG:HH11	1:G:332:HIS:CD2	2.15	0.64
1:F:255:ALA:O	1:F:259:GLN:HB2	1.97	0.64
1:G:228:THR:HG23	1:G:229:ASP:OD2	1.98	0.64
1:A:173:THR:HG22	1:A:205:ALA:HB3	1.80	0.64
1:B:324:ILE:HD12	1:B:338:ALA:O	1.98	0.64
1:G:196:VAL:C	1:G:198:LYS:H	2.05	0.64
1:A:37:ILE:HD13	1:A:38:GLU:H	1.63	0.63
1:A:254:LEU:HD22	1:B:249:ILE:HD11	1.80	0.63
1:G:188:ASN:O	1:G:345:LYS:HE2	1.98	0.63
1:F:146:GLN:HA	1:F:146:GLN:NE2	2.13	0.63
1:B:257:ARG:O	1:B:261:LEU:HB2	1.98	0.63
1:D:186:ALA:CB	1:D:196:VAL:HG21	2.28	0.63
1:F:251:ARG:N	1:F:251:ARG:HD3	2.11	0.63
1:A:69:GLU:O	1:A:73:VAL:HG23	1.99	0.63
1:C:317:LYS:HG3	1:C:323:ARG:HH12	1.64	0.63
1:F:190:GLY:O	1:F:191:LEU:HD23	1.98	0.63
1:A:146:GLN:HE21	1:A:146:GLN:HA	1.63	0.63
1:F:177:PHE:CD2	1:F:202:VAL:HG11	2.34	0.63
4:F:373:GOL:C1	4:F:373:GOL:HO1	2.09	0.63
1:E:304:ILE:HG12	1:E:305:LEU:H	1.63	0.63
1:G:187:GLN:HB3	1:G:193:PRO:CG	2.29	0.63
1:G:327:LEU:HD12	1:G:327:LEU:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLN:HE21	1:A:264:HIS:CE1	2.17	0.62
1:F:328:ILE:O	1:F:328:ILE:HG22	1.98	0.62
1:G:330:ALA:HB3	1:G:331:PRO:HD3	1.81	0.62
1:C:317:LYS:HG3	1:C:323:ARG:NH1	2.13	0.62
1:F:99:ARG:HB3	1:F:102:GLU:HG2	1.80	0.62
1:A:259:GLN:NE2	1:B:247:GLU:HB3	2.15	0.62
1:F:251:ARG:C	1:F:253:ALA:H	2.07	0.62
1:G:170:TRP:HB3	1:G:202:VAL:CG1	2.29	0.62
1:A:188:ASN:ND2	1:A:344:GLU:CB	2.63	0.62
1:B:146:GLN:HA	1:B:146:GLN:NE2	2.14	0.62
1:D:189:ARG:NH2	1:D:345:LYS:HB3	2.13	0.62
1:E:146:GLN:HA	1:E:146:GLN:NE2	2.14	0.62
1:E:146:GLN:HE22	1:E:181:ARG:HE	1.48	0.62
1:A:37:ILE:CD1	1:A:52:ARG:HH12	2.13	0.62
1:C:218:ALA:O	1:C:222:ILE:HG13	1.99	0.62
1:F:146:GLN:HE22	1:F:181:ARG:HE	1.46	0.62
1:F:101:ASP:OD2	1:F:102:GLU:N	2.33	0.62
1:G:144:LYS:HG2	2:G:356:SO4:O2	1.99	0.61
1:A:170:TRP:HB3	1:A:202:VAL:HG12	1.82	0.61
1:C:181:ARG:O	1:C:185:ILE:HG12	2.00	0.61
1:G:327:LEU:HD12	1:G:327:LEU:H	1.65	0.61
1:A:171:ILE:CD1	1:G:97:PHE:HE1	2.13	0.61
1:A:219:GLU:O	1:A:223:LYS:HG2	2.00	0.61
1:D:190:GLY:O	1:D:191:LEU:HB2	2.01	0.61
1:D:222:ILE:HD13	1:D:222:ILE:N	2.16	0.61
1:E:137:PHE:CZ	1:E:314:TYR:HB2	2.35	0.61
1:E:330:ALA:N	1:E:331:PRO:HD2	1.98	0.61
1:G:228:THR:HG22	1:G:230:ARG:H	1.65	0.61
1:C:118:LYS:HB2	1:C:349:ASP:OD1	1.99	0.61
1:C:156:GLN:OE1	1:C:199:HIS:HB2	2.01	0.61
1:F:221:LYS:HZ3	3:F:363:IMD:H4	1.65	0.61
1:A:159:PRO:HD3	1:A:165:ASN:ND2	2.15	0.61
1:E:96:THR:HG22	1:E:97:PHE:HD1	1.65	0.61
1:A:157:LEU:HD13	1:A:161:GLU:HB2	1.80	0.61
1:D:185:ILE:HG23	1:D:345:LYS:HA	1.82	0.61
1:G:173:THR:HG22	1:G:205:ALA:HB3	1.81	0.61
1:A:177:PHE:CD2	1:A:202:VAL:HG11	2.35	0.61
1:A:252:GLY:CA	1:G:251:ARG:HH22	2.13	0.61
1:B:187:GLN:C	1:B:189:ARG:H	2.09	0.61
1:A:251:ARG:HG3	1:A:251:ARG:HH11	1.65	0.61
1:E:344:GLU:O	1:E:345:LYS:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:HD2	1:G:332:HIS:NE2	2.16	0.60
1:D:274:LEU:HD12	1:D:275:TYR:CZ	2.36	0.60
1:B:183:ARG:HG3	1:B:193:PRO:HB2	1.83	0.60
1:C:146:GLN:HA	1:C:146:GLN:NE2	2.16	0.60
1:E:119:SER:HB2	1:E:349:ASP:OD1	2.01	0.60
1:F:98:MSE:CG	1:F:102:GLU:HB2	2.31	0.60
1:G:274:LEU:HD12	1:G:275:TYR:CZ	2.36	0.60
1:A:331:PRO:HD3	1:B:140:PHE:HZ	1.67	0.60
1:E:257:ARG:NH2	1:E:304:ILE:HB	2.17	0.60
1:F:105:LYS:HG3	1:F:106:LYS:N	2.16	0.60
1:C:274:LEU:HD12	1:C:275:TYR:CZ	2.37	0.60
1:E:333:LEU:HG	1:E:334:PRO:HD2	1.84	0.60
1:G:113:ILE:CD1	1:G:164:LEU:HD23	2.32	0.60
1:G:274:LEU:HD13	1:G:274:LEU:O	2.01	0.60
1:G:328:ILE:N	1:G:328:ILE:HD12	2.16	0.60
1:A:113:ILE:CD1	1:A:164:LEU:HG	2.32	0.60
1:E:201:TYR:CD2	1:E:221:LYS:HE2	2.37	0.60
1:C:111:GLY:HA3	6:C:404:HOH:O	2.00	0.60
1:D:330:ALA:H	1:D:331:PRO:CD	2.10	0.59
1:F:215:VAL:HG21	1:F:264:HIS:NE2	2.16	0.59
1:F:286:GLN:H	1:F:286:GLN:CD	2.09	0.59
1:A:82:LEU:HD13	1:A:82:LEU:C	2.27	0.59
1:D:263:LYS:NZ	1:D:263:LYS:HB3	2.17	0.59
1:A:221:LYS:O	1:A:225:LEU:HD13	2.02	0.59
1:C:196:VAL:C	1:C:198:LYS:H	2.09	0.59
1:D:183:ARG:C	1:D:185:ILE:H	2.10	0.59
1:D:223:LYS:HB2	1:D:223:LYS:NZ	2.17	0.59
1:C:251:ARG:HA	1:C:254:LEU:HB3	1.84	0.59
1:D:225:LEU:HD12	1:D:225:LEU:N	2.17	0.59
1:D:326:ARG:HG2	1:D:327:LEU:N	2.18	0.59
1:A:42:GLY:HA3	1:A:84:ILE:HD11	1.85	0.59
1:B:255:ALA:O	1:B:259:GLN:HG2	2.02	0.59
1:F:332:HIS:CE1	1:G:178:ARG:HH11	2.19	0.59
1:B:316:ARG:HH12	1:B:326:ARG:HH21	1.49	0.59
1:E:146:GLN:HG3	1:E:342:ILE:HD12	1.84	0.59
1:G:146:GLN:HA	1:G:146:GLN:NE2	2.17	0.59
1:D:121:ASP:O	1:D:126:GLY:N	2.32	0.59
1:E:257:ARG:CZ	1:E:304:ILE:HB	2.32	0.59
1:A:317:LYS:HE2	1:A:323:ARG:HH22	1.68	0.58
1:B:228:THR:HG22	1:B:230:ARG:N	2.02	0.58
1:C:117:SER:HB3	1:C:347:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLN:HA	1:D:146:GLN:NE2	2.16	0.58
1:E:185:ILE:HG12	1:E:346:GLY:N	2.18	0.58
1:E:328:ILE:O	1:E:329:ASP:CB	2.51	0.58
1:G:223:LYS:O	1:G:225:LEU:N	2.35	0.58
1:C:285:VAL:O	1:C:286:GLN:CB	2.51	0.58
1:D:326:ARG:HB3	1:D:326:ARG:NH2	2.13	0.58
1:B:100:ALA:HB1	1:C:197:LEU:HD13	1.85	0.58
1:D:344:GLU:O	1:D:345:LYS:HB2	2.03	0.58
1:F:98:MSE:HG2	1:F:102:GLU:HB2	1.85	0.58
1:B:177:PHE:HE1	1:B:182:ILE:HD12	1.69	0.58
1:D:235:LEU:C	1:D:235:LEU:HD23	2.29	0.58
1:E:184:GLU:O	1:E:188:ASN:HB2	2.03	0.58
1:B:314:TYR:N	1:B:328:ILE:HD11	2.19	0.58
1:F:170:TRP:HB3	1:F:202:VAL:CG1	2.33	0.58
1:G:112:ARG:HD3	1:G:126:GLY:HA3	1.86	0.58
1:C:213:LEU:O	1:C:213:LEU:HD23	2.04	0.58
1:D:113:ILE:HD11	1:D:164:LEU:HD12	1.84	0.58
1:B:184:GLU:HG2	6:B:386:HOH:O	2.03	0.58
1:D:303:HIS:HE1	1:D:305:LEU:HD13	1.69	0.58
4:D:369:GOL:C1	4:D:369:GOL:HO1	2.08	0.58
1:B:156:GLN:OE1	1:B:199:HIS:HB2	2.04	0.58
1:G:156:GLN:OE1	1:G:199:HIS:HB2	2.04	0.58
1:A:258:GLN:HG3	1:B:249:ILE:HD12	1.83	0.58
1:B:314:TYR:HB2	1:B:328:ILE:HD11	1.86	0.58
1:C:185:ILE:HA	6:C:384:HOH:O	2.04	0.58
1:F:104:LEU:HD12	1:G:180:GLU:HG3	1.85	0.58
1:A:228:THR:HG22	1:A:229:ASP:N	2.18	0.57
1:B:159:PRO:HD3	1:B:165:ASN:ND2	2.19	0.57
1:E:213:LEU:HD22	1:E:213:LEU:O	2.04	0.57
1:G:160:GLU:CD	1:G:160:GLU:H	2.12	0.57
1:B:187:GLN:HG3	1:B:188:ASN:N	2.18	0.57
1:E:225:LEU:N	1:E:225:LEU:HD12	2.19	0.57
1:A:344:GLU:O	1:A:345:LYS:HB2	2.05	0.57
1:B:99:ARG:HE	1:C:198:LYS:HA	1.67	0.57
1:C:191:LEU:N	1:C:191:LEU:HD12	2.19	0.57
1:E:159:PRO:HD3	1:E:165:ASN:ND2	2.18	0.57
1:A:328:ILE:O	1:A:329:ASP:HB3	2.04	0.57
1:F:137:PHE:CZ	1:F:314:TYR:HB2	2.39	0.57
1:A:330:ALA:N	1:A:331:PRO:CD	2.65	0.57
1:B:316:ARG:NH1	1:B:326:ARG:HH21	2.02	0.57
1:C:181:ARG:NH2	1:C:185:ILE:CD1	2.65	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:MSE:SE	1:D:189:ARG:HH11	2.38	0.57
1:E:322:LYS:NZ	1:E:341:SER:HB3	2.18	0.57
1:D:177:PHE:CE1	1:D:182:ILE:HD11	2.38	0.57
1:A:37:ILE:HD11	1:A:52:ARG:NH1	2.17	0.57
1:B:332:HIS:HB3	1:B:333:LEU:HD12	1.86	0.57
1:C:99:ARG:HH22	4:C:368:GOL:H12	1.69	0.57
1:D:139:GLU:HG2	1:D:286:GLN:HB3	1.86	0.57
1:D:329:ASP:CG	1:D:330:ALA:N	2.57	0.57
1:C:226:LEU:HA	1:C:231:PRO:HB3	1.87	0.57
1:D:170:TRP:HB3	1:D:202:VAL:CG1	2.34	0.57
1:A:211:GLN:HE21	1:A:264:HIS:HE1	1.51	0.57
1:B:323:ARG:HH21	1:B:323:ARG:HG3	1.69	0.57
1:A:320:GLY:HA2	3:A:361:IMD:N3	2.20	0.56
1:D:146:GLN:HG3	1:D:342:ILE:HD12	1.87	0.56
1:D:332:HIS:O	1:D:333:LEU:HD22	2.05	0.56
1:F:170:TRP:HB3	1:F:202:VAL:HG12	1.86	0.56
1:A:37:ILE:HG12	1:A:38:GLU:H	1.69	0.56
1:A:274:LEU:HD12	1:A:275:TYR:CZ	2.40	0.56
1:A:123:LEU:HG	1:A:327:LEU:HD13	1.86	0.56
1:A:213:LEU:O	1:A:216:GLN:HG2	2.05	0.56
1:A:274:LEU:HD13	1:A:274:LEU:O	2.04	0.56
1:B:101:ASP:CG	1:B:102:GLU:N	2.63	0.56
1:F:157:LEU:HD13	1:F:161:GLU:CB	2.34	0.56
1:G:329:ASP:O	1:G:330:ALA:HB2	2.05	0.56
1:B:322:LYS:C	1:B:323:ARG:HD2	2.31	0.56
1:D:156:GLN:OE1	1:D:199:HIS:HB2	2.05	0.56
1:B:322:LYS:NZ	1:B:341:SER:HB3	2.20	0.56
1:C:286:GLN:HE21	1:C:286:GLN:HA	1.70	0.56
1:F:169:ILE:HD11	1:F:221:LYS:CG	2.35	0.56
1:F:228:THR:HG22	1:F:230:ARG:H	1.70	0.56
1:E:235:LEU:HD23	1:E:235:LEU:C	2.31	0.56
1:E:333:LEU:CG	1:E:334:PRO:HD2	2.36	0.56
1:E:344:GLU:O	1:E:345:LYS:CB	2.54	0.56
1:B:149:HIS:HD2	1:B:182:ILE:HG13	1.70	0.56
1:G:97:PHE:N	1:G:97:PHE:CD2	2.72	0.56
1:G:185:ILE:HG13	1:G:345:LYS:C	2.31	0.56
1:G:211:GLN:HE21	1:G:264:HIS:CE1	2.24	0.56
1:A:188:ASN:ND2	1:A:344:GLU:HB3	2.21	0.56
1:D:190:GLY:O	1:D:191:LEU:CB	2.53	0.56
1:F:159:PRO:HD3	1:F:165:ASN:ND2	2.21	0.56
1:C:188:ASN:OD1	1:C:344:GLU:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:344:GLU:O	1:G:345:LYS:HB2	2.05	0.56
1:A:163:GLY:O	1:A:164:LEU:HD23	2.04	0.55
1:A:286:GLN:HA	1:A:286:GLN:NE2	2.20	0.55
1:B:211:GLN:HE21	1:B:264:HIS:HE1	1.54	0.55
1:F:175:ASN:H	1:F:204:ARG:NH1	2.03	0.55
1:A:147:LEU:HD22	1:A:151:LEU:HD22	1.88	0.55
1:B:211:GLN:HE21	1:B:264:HIS:CE1	2.24	0.55
1:E:98:MSE:HG3	1:E:102:GLU:OE1	2.06	0.55
1:D:187:GLN:HB3	1:D:193:PRO:CD	2.28	0.55
1:G:314:TYR:HB3	1:G:328:ILE:HD11	1.89	0.55
1:A:37:ILE:CG1	1:A:38:GLU:N	2.69	0.55
1:A:81:ALA:O	1:A:85:ILE:HG12	2.06	0.55
1:B:177:PHE:CD2	1:B:202:VAL:HG11	2.42	0.55
1:D:326:ARG:HH21	1:D:326:ARG:CB	2.12	0.55
1:E:324:ILE:HD11	1:E:337:GLU:HB3	1.89	0.55
1:F:330:ALA:N	1:F:331:PRO:HD2	2.21	0.55
1:B:344:GLU:O	1:B:345:LYS:HB2	2.07	0.55
1:C:258:GLN:O	1:C:259:GLN:C	2.49	0.55
1:A:171:ILE:HD11	1:G:97:PHE:HE1	1.71	0.55
1:E:274:LEU:HD13	1:E:274:LEU:O	2.06	0.55
1:F:344:GLU:O	1:F:345:LYS:HB2	2.05	0.55
1:D:330:ALA:N	1:D:331:PRO:CD	2.68	0.55
1:E:156:GLN:HE22	1:E:196:VAL:HG13	1.68	0.55
1:G:225:LEU:HG	1:G:231:PRO:HA	1.89	0.55
1:D:332:HIS:ND1	6:D:399:HOH:O	2.34	0.54
1:F:274:LEU:HD13	1:F:274:LEU:O	2.07	0.54
1:A:118:LYS:O	1:A:122:LYS:HG3	2.07	0.54
1:A:286:GLN:HA	1:A:286:GLN:HE21	1.72	0.54
1:D:225:LEU:O	1:D:231:PRO:HA	2.06	0.54
1:G:245:ARG:O	1:G:245:ARG:HG3	2.08	0.54
1:C:344:GLU:O	1:C:345:LYS:HB2	2.06	0.54
1:D:185:ILE:HG23	1:D:345:LYS:CA	2.38	0.54
1:E:113:ILE:HD11	1:E:164:LEU:HD12	1.90	0.54
1:F:157:LEU:O	1:F:163:GLY:HA3	2.07	0.54
1:F:157:LEU:HD12	1:F:163:GLY:N	2.22	0.54
1:A:113:ILE:N	1:A:113:ILE:HD13	2.22	0.54
1:C:97:PHE:CD1	1:C:97:PHE:N	2.74	0.54
1:F:219:GLU:CD	1:F:270:ARG:HH22	2.14	0.54
1:F:324:ILE:HD13	1:F:324:ILE:C	2.33	0.54
1:G:223:LYS:HB2	1:G:223:LYS:NZ	2.23	0.54
1:C:128:ILE:HG13	1:C:128:ILE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:GLY:O	1:F:319:LYS:C	2.51	0.54
1:C:196:VAL:O	1:C:198:LYS:N	2.41	0.54
1:D:274:LEU:HD13	1:D:274:LEU:O	2.07	0.54
1:F:192:ASP:HB3	1:F:195:GLU:HB2	1.89	0.54
1:B:119:SER:N	1:B:349:ASP:OD1	2.40	0.54
1:C:274:LEU:HD13	1:C:274:LEU:O	2.08	0.54
1:C:330:ALA:N	1:C:331:PRO:CD	2.70	0.54
1:E:225:LEU:HD12	1:E:225:LEU:H	1.72	0.54
1:G:196:VAL:O	1:G:198:LYS:N	2.40	0.54
1:A:225:LEU:N	1:A:225:LEU:HD12	2.23	0.54
1:D:142:SER:O	1:D:315:LEU:HD13	2.08	0.54
1:D:212:MSE:HE1	1:D:260:LYS:HE2	1.90	0.54
1:A:146:GLN:HA	1:A:146:GLN:NE2	2.23	0.53
1:A:146:GLN:HG3	1:A:342:ILE:HD12	1.90	0.53
1:A:215:VAL:HG11	1:A:267:ASP:HB3	1.89	0.53
1:C:286:GLN:HA	1:C:286:GLN:NE2	2.23	0.53
1:F:185:ILE:HG23	1:F:345:LYS:C	2.32	0.53
1:B:117:SER:OG	1:B:349:ASP:HA	2.08	0.53
1:B:184:GLU:O	1:B:187:GLN:HG2	2.09	0.53
1:C:230:ARG:HG2	1:C:230:ARG:HH11	1.72	0.53
1:G:327:LEU:H	1:G:327:LEU:CD1	2.21	0.53
1:C:328:ILE:HG22	1:C:328:ILE:O	2.07	0.53
1:E:170:TRP:HB3	1:E:202:VAL:HG12	1.89	0.53
1:F:214:LEU:HD12	1:F:217:GLN:OE1	2.08	0.53
1:B:99:ARG:NH2	1:C:198:LYS:HG2	2.23	0.53
1:B:212:MSE:HE1	1:B:260:LYS:CD	2.36	0.53
1:C:142:SER:O	1:C:315:LEU:HD13	2.09	0.53
1:D:113:ILE:CD1	1:D:164:LEU:HD12	2.38	0.53
1:G:137:PHE:CZ	1:G:314:TYR:HB2	2.43	0.53
1:A:52:ARG:C	1:A:54:ALA:H	2.16	0.53
1:A:99:ARG:HH22	4:B:367:GOL:H12	1.73	0.53
1:B:252:GLY:N	3:B:359:IMD:N3	2.56	0.53
1:C:101:ASP:OD1	1:C:102:GLU:N	2.41	0.53
1:D:323:ARG:H	1:D:323:ARG:HD2	1.73	0.53
1:A:146:GLN:HE22	1:A:181:ARG:HE	1.56	0.53
1:B:137:PHE:CZ	1:B:314:TYR:HB2	2.42	0.53
1:D:167:SER:OG	1:D:225:LEU:HD23	2.08	0.53
1:E:324:ILE:HD13	1:E:324:ILE:C	2.34	0.53
1:F:265:LEU:HD21	1:F:306:ALA:HA	1.90	0.53
1:A:249:ILE:N	1:A:249:ILE:CD1	2.63	0.53
1:D:154:MSE:SE	1:D:189:ARG:NH1	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:TRP:HB3	1:D:202:VAL:HG12	1.91	0.53
1:G:146:GLN:HG3	1:G:342:ILE:HD12	1.90	0.53
1:G:255:ALA:O	1:G:259:GLN:HG2	2.08	0.53
1:A:42:GLY:CA	1:A:84:ILE:HD11	2.38	0.53
1:G:257:ARG:NH1	1:G:304:ILE:HD13	2.24	0.53
1:C:103:TYR:CE1	1:C:107:ARG:HD2	2.44	0.53
1:G:108:ALA:C	1:G:110:ILE:H	2.17	0.53
1:B:157:LEU:HD13	1:B:161:GLU:HB3	1.90	0.53
1:D:107:ARG:HD3	1:E:180:GLU:OE2	2.09	0.53
1:D:182:ILE:HB	1:D:197:LEU:HD21	1.91	0.53
1:E:142:SER:O	1:E:315:LEU:HD13	2.09	0.53
1:E:181:ARG:NH1	1:E:346:GLY:HA2	2.23	0.53
1:F:146:GLN:HG3	1:F:342:ILE:HD12	1.91	0.53
1:B:237:VAL:HB	1:B:281:VAL:HG12	1.92	0.52
1:B:320:GLY:HA2	3:B:360:IMD:HN3	1.74	0.52
1:D:183:ARG:O	1:D:185:ILE:N	2.42	0.52
1:F:226:LEU:C	1:F:226:LEU:HD13	2.34	0.52
1:A:82:LEU:O	1:A:86:GLN:HG3	2.09	0.52
1:A:170:TRP:HB3	1:A:202:VAL:CG1	2.39	0.52
1:A:251:ARG:HG2	1:B:251:ARG:HG2	1.92	0.52
1:A:324:ILE:HD13	1:A:337:GLU:HB3	1.89	0.52
1:C:187:GLN:HA	1:C:191:LEU:O	2.10	0.52
1:C:235:LEU:HD23	1:C:235:LEU:C	2.34	0.52
1:D:222:ILE:N	1:D:222:ILE:CD1	2.72	0.52
1:D:225:LEU:HD12	1:D:225:LEU:H	1.74	0.52
1:E:123:LEU:HG	1:E:327:LEU:HD13	1.91	0.52
1:G:245:ARG:HH22	1:G:283:ASN:HD21	1.58	0.52
1:D:305:LEU:HD23	1:D:305:LEU:O	2.09	0.52
1:D:316:ARG:NH1	1:D:337:GLU:OE2	2.39	0.52
1:A:158:PRO:HD2	1:A:161:GLU:HG3	1.91	0.52
1:B:99:ARG:NE	1:C:198:LYS:HA	2.23	0.52
1:B:112:ARG:HD3	1:B:126:GLY:HA3	1.92	0.52
1:D:183:ARG:C	1:D:185:ILE:N	2.68	0.52
1:D:192:ASP:OD2	1:D:195:GLU:HB2	2.09	0.52
1:A:179:PRO:HG2	1:G:104:LEU:HD13	1.92	0.52
1:A:222:ILE:HD13	1:A:277:ILE:CD1	2.40	0.52
1:B:252:GLY:N	3:B:359:IMD:HN3	2.07	0.52
1:C:214:LEU:HA	1:C:217:GLN:OE1	2.10	0.52
1:D:344:GLU:O	1:D:345:LYS:CB	2.58	0.52
1:A:184:GLU:O	1:A:186:ALA:N	2.43	0.52
1:B:329:ASP:O	1:B:330:ALA:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:HIS:HB3	1:B:333:LEU:CD1	2.39	0.52
1:C:184:GLU:HG2	6:C:384:HOH:O	2.10	0.52
1:C:225:LEU:O	1:C:231:PRO:HA	2.08	0.52
1:F:104:LEU:HB2	1:G:179:PRO:CG	2.40	0.52
1:G:164:LEU:O	1:G:165:ASN:C	2.52	0.52
1:D:326:ARG:NH2	1:D:326:ARG:CB	2.72	0.52
1:G:318:GLY:N	1:G:322:LYS:O	2.31	0.52
1:A:254:LEU:HD13	1:B:249:ILE:HG12	1.92	0.52
1:B:304:ILE:HD13	1:B:304:ILE:C	2.34	0.52
1:C:137:PHE:CZ	1:C:314:TYR:HB2	2.45	0.52
1:C:304:ILE:CG1	1:C:305:LEU:N	2.73	0.52
1:A:165:ASN:HA	1:A:230:ARG:HH12	1.75	0.51
1:E:105:LYS:O	1:E:108:ALA:HB3	2.09	0.51
1:E:207:ASN:HB2	1:E:247:GLU:OE1	2.10	0.51
1:E:230:ARG:HB3	1:E:230:ARG:HH11	1.75	0.51
1:F:316:ARG:HG2	1:F:324:ILE:HG22	1.92	0.51
1:A:331:PRO:CD	1:B:140:PHE:HZ	2.23	0.51
1:B:302:GLY:C	1:B:304:ILE:N	2.67	0.51
1:C:211:GLN:HE21	1:C:264:HIS:CE1	2.28	0.51
1:E:170:TRP:HB3	1:E:202:VAL:CG1	2.40	0.51
1:F:344:GLU:O	1:F:345:LYS:CB	2.58	0.51
1:A:249:ILE:CD1	1:G:258:GLN:HG3	2.40	0.51
1:B:183:ARG:CG	1:B:193:PRO:HB2	2.40	0.51
1:C:211:GLN:HE21	1:C:264:HIS:HE1	1.57	0.51
1:F:332:HIS:O	1:F:333:LEU:HB2	2.10	0.51
1:G:207:ASN:HB2	1:G:247:GLU:OE1	2.10	0.51
1:B:254:LEU:H	3:B:359:IMD:H4	1.75	0.51
1:B:322:LYS:HZ3	1:B:341:SER:HB3	1.76	0.51
1:C:323:ARG:HE	1:C:342:ILE:HG13	1.75	0.51
1:F:180:GLU:H	1:F:180:GLU:CD	2.18	0.51
1:G:195:GLU:O	1:G:198:LYS:HB2	2.11	0.51
1:A:317:LYS:HE2	1:A:323:ARG:NH2	2.26	0.51
1:A:344:GLU:O	1:A:345:LYS:CB	2.58	0.51
1:B:99:ARG:HH21	1:C:198:LYS:HG2	1.75	0.51
1:B:320:GLY:HA2	3:B:360:IMD:N3	2.25	0.51
1:F:218:ALA:O	1:F:220:ASP:N	2.43	0.51
1:F:332:HIS:C	1:F:333:LEU:HD12	2.35	0.51
1:D:114:SER:CA	1:D:121:ASP:OD2	2.58	0.51
1:G:117:SER:HB2	1:G:349:ASP:OXT	2.11	0.51
1:G:133:ILE:HD13	1:G:269:HIS:ND1	2.26	0.51
1:G:235:LEU:C	1:G:235:LEU:HD23	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ILE:HD12	1:D:214:LEU:HB3	1.92	0.51
1:D:177:PHE:HE1	1:D:182:ILE:HD11	1.73	0.51
1:F:235:LEU:C	1:F:235:LEU:HD23	2.35	0.51
1:G:124:LEU:O	1:G:333:LEU:HD21	2.10	0.51
1:B:182:ILE:HG22	1:B:183:ARG:N	2.26	0.51
1:D:99:ARG:NE	1:D:101:ASP:OD2	2.41	0.51
1:D:128:ILE:HG13	1:D:128:ILE:O	2.09	0.51
1:E:118:LYS:N	1:E:349:ASP:OD2	2.44	0.51
1:G:316:ARG:NH1	1:G:337:GLU:OE2	2.42	0.51
1:A:169:ILE:HD11	1:A:221:LYS:HG2	1.93	0.51
1:A:241:THR:OG1	1:A:283:ASN:ND2	2.44	0.51
1:B:146:GLN:HG3	1:B:342:ILE:HD12	1.92	0.51
1:B:178:ARG:HB2	1:B:181:ARG:HB3	1.93	0.51
1:B:251:ARG:O	1:B:253:ALA:N	2.44	0.51
1:F:258:GLN:HE21	1:F:258:GLN:CA	2.00	0.51
1:B:142:SER:O	1:B:315:LEU:HD13	2.11	0.51
1:B:235:LEU:C	1:B:235:LEU:HD23	2.36	0.51
1:F:179:PRO:HG2	1:F:180:GLU:OE2	2.11	0.50
1:F:237:VAL:HB	1:F:281:VAL:HG12	1.92	0.50
1:G:142:SER:O	1:G:315:LEU:HD13	2.11	0.50
1:C:225:LEU:C	1:C:231:PRO:HA	2.35	0.50
1:E:316:ARG:NH1	1:E:324:ILE:HD12	2.27	0.50
1:F:184:GLU:OE2	1:F:344:GLU:HA	2.11	0.50
1:G:187:GLN:O	1:G:187:GLN:HG3	2.12	0.50
1:A:37:ILE:HG12	1:A:38:GLU:N	2.26	0.50
1:A:212:MSE:HE1	1:A:260:LYS:CD	2.36	0.50
1:A:331:PRO:HD3	1:B:140:PHE:CZ	2.46	0.50
1:B:177:PHE:CE1	1:B:182:ILE:HD12	2.46	0.50
1:C:187:GLN:HB3	1:C:193:PRO:CD	2.40	0.50
1:D:207:ASN:HA	1:D:243:HIS:ND1	2.27	0.50
1:E:120:LEU:HD22	1:E:124:LEU:CD1	2.41	0.50
1:G:215:VAL:HG21	1:G:264:HIS:NE2	2.26	0.50
1:B:101:ASP:OD1	1:B:102:GLU:N	2.44	0.50
1:B:274:LEU:HD12	1:B:275:TYR:CE2	2.47	0.50
1:F:322:LYS:O	1:F:323:ARG:NH1	2.44	0.50
1:A:304:ILE:HG13	1:A:305:LEU:N	2.27	0.50
1:D:223:LYS:HB2	1:D:223:LYS:HZ3	1.75	0.50
1:D:252:GLY:HA2	6:D:385:HOH:O	2.11	0.50
1:D:327:LEU:CD1	1:D:333:LEU:HB3	2.42	0.50
1:A:142:SER:O	1:A:315:LEU:HD13	2.11	0.50
1:A:228:THR:HG22	1:A:230:ARG:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLN:HG3	1:A:286:GLN:O	2.12	0.50
1:B:219:GLU:CD	1:B:270:ARG:NH2	2.69	0.50
1:D:137:PHE:CZ	1:D:314:TYR:HB2	2.46	0.50
1:F:100:ALA:HB3	1:G:197:LEU:HA	1.94	0.50
1:F:101:ASP:OD2	1:F:102:GLU:HG2	2.10	0.50
1:B:330:ALA:N	1:B:331:PRO:HD2	2.15	0.50
1:F:330:ALA:H	1:F:331:PRO:HD2	1.75	0.50
1:G:106:LYS:C	1:G:108:ALA:H	2.20	0.50
1:G:187:GLN:HB3	1:G:193:PRO:HG3	1.92	0.50
1:B:248:TYR:OH	1:B:260:LYS:HD2	2.12	0.50
1:B:344:GLU:O	1:B:345:LYS:CB	2.60	0.50
1:C:146:GLN:HG3	1:C:342:ILE:HD12	1.93	0.50
1:G:178:ARG:O	1:G:181:ARG:HB3	2.11	0.50
1:D:112:ARG:HD2	1:D:126:GLY:HA3	1.93	0.50
1:A:37:ILE:HG23	1:A:39:ASP:OD2	2.12	0.49
1:B:158:PRO:O	1:B:161:GLU:HB2	2.12	0.49
1:C:269:HIS:HB3	1:D:206:PHE:CD2	2.47	0.49
1:E:99:ARG:HE	1:F:198:LYS:HA	1.77	0.49
1:E:156:GLN:OE1	1:E:199:HIS:HB2	2.12	0.49
1:E:274:LEU:HD12	1:E:275:TYR:CE2	2.47	0.49
1:A:107:ARG:HH21	1:B:178:ARG:CZ	2.25	0.49
1:A:215:VAL:O	1:A:218:ALA:HB3	2.11	0.49
1:B:182:ILE:O	1:B:183:ARG:C	2.54	0.49
1:D:326:ARG:HG2	1:D:327:LEU:H	1.76	0.49
1:F:169:ILE:HD11	1:F:221:LYS:HG2	1.94	0.49
1:C:230:ARG:HG2	1:C:230:ARG:NH1	2.27	0.49
1:A:164:LEU:O	1:A:165:ASN:C	2.56	0.49
1:A:257:ARG:NH2	1:A:304:ILE:HD13	2.27	0.49
1:A:264:HIS:HD2	6:A:429:HOH:O	1.94	0.49
1:A:318:GLY:O	1:A:319:LYS:C	2.54	0.49
1:B:146:GLN:HE21	1:B:146:GLN:CA	2.20	0.49
1:B:254:LEU:HD21	1:C:249:ILE:HG21	1.94	0.49
1:C:160:GLU:CD	1:C:160:GLU:H	2.20	0.49
1:C:324:ILE:HD11	1:C:337:GLU:HB3	1.93	0.49
1:E:192:ASP:HB3	1:E:195:GLU:HB2	1.94	0.49
1:F:201:TYR:CD1	1:F:201:TYR:N	2.81	0.49
1:F:304:ILE:HG22	1:F:305:LEU:N	2.27	0.49
1:G:330:ALA:HB3	1:G:331:PRO:CD	2.41	0.49
1:G:348:GLU:O	1:G:349:ASP:CB	2.57	0.49
1:B:97:PHE:O	1:B:98:MSE:C	2.56	0.49
1:F:166:GLY:HA3	1:F:233:LYS:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:PRO:O	1:G:182:ILE:HB	2.13	0.49
1:G:184:GLU:HG2	1:G:185:ILE:N	2.27	0.49
1:G:327:LEU:C	1:G:328:ILE:HD12	2.37	0.49
1:C:181:ARG:HH21	1:C:181:ARG:HG3	1.76	0.49
1:D:142:SER:O	1:D:323:ARG:HG2	2.12	0.49
1:E:145:THR:HG23	1:E:238:ASP:OD2	2.13	0.49
1:A:118:LYS:N	1:A:349:ASP:OXT	2.46	0.49
1:C:330:ALA:H	1:C:331:PRO:CD	2.17	0.49
1:E:120:LEU:HD22	1:E:124:LEU:HD11	1.94	0.49
1:E:254:LEU:HD12	1:E:254:LEU:O	2.13	0.49
1:F:157:LEU:HD12	1:F:163:GLY:H	1.77	0.49
1:A:52:ARG:C	1:A:54:ALA:N	2.71	0.49
1:A:326:ARG:HD3	1:A:337:GLU:CG	2.37	0.49
1:C:185:ILE:HD13	6:C:384:HOH:O	2.12	0.49
1:G:201:TYR:N	1:G:201:TYR:CD1	2.80	0.49
1:B:160:GLU:CD	1:B:160:GLU:H	2.20	0.49
1:E:118:LYS:HB2	1:E:349:ASP:OD2	2.12	0.49
1:E:133:ILE:HD13	1:E:269:HIS:ND1	2.28	0.49
1:A:348:GLU:O	1:A:349:ASP:HB2	2.12	0.49
1:B:249:ILE:HD13	1:B:249:ILE:H	1.78	0.49
1:B:316:ARG:NH1	1:B:326:ARG:NH2	2.61	0.49
1:B:328:ILE:N	1:B:328:ILE:CD1	2.70	0.49
1:C:188:ASN:OD1	1:C:344:GLU:CB	2.61	0.49
1:C:250:GLY:O	1:C:253:ALA:HB3	2.12	0.49
1:D:214:LEU:O	1:D:218:ALA:HB2	2.13	0.49
1:F:144:LYS:HG2	2:F:355:SO4:O4	2.12	0.49
1:D:245:ARG:NH1	1:D:304:ILE:HG22	2.28	0.48
1:F:99:ARG:HD2	1:G:198:LYS:O	2.12	0.48
1:F:250:GLY:O	1:F:253:ALA:HB3	2.12	0.48
1:D:101:ASP:OD1	1:D:102:GLU:N	2.45	0.48
1:F:147:LEU:HA	1:F:347:ILE:CD1	2.43	0.48
1:F:333:LEU:HB3	1:F:334:PRO:HD2	1.96	0.48
1:G:160:GLU:N	1:G:160:GLU:OE1	2.46	0.48
1:G:332:HIS:O	1:G:333:LEU:CB	2.53	0.48
1:A:241:THR:HB	1:A:304:ILE:HG21	1.95	0.48
1:D:263:LYS:HB3	1:D:263:LYS:HZ2	1.77	0.48
1:B:123:LEU:CD1	1:B:334:PRO:HG2	2.42	0.48
1:B:189:ARG:HG3	1:B:345:LYS:HG2	1.96	0.48
1:B:326:ARG:HG2	1:B:327:LEU:N	2.28	0.48
1:B:205:ALA:O	1:B:243:HIS:HE1	1.97	0.48
1:B:314:TYR:HB3	1:B:328:ILE:HD11	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ILE:HD13	1:D:200:ILE:CD1	2.41	0.48
1:C:117:SER:HB2	1:C:349:ASP:OD2	2.13	0.48
1:C:147:LEU:HD22	1:C:151:LEU:HD22	1.96	0.48
1:C:166:GLY:HA3	1:C:233:LYS:HG3	1.96	0.48
1:C:225:LEU:H	1:C:225:LEU:CD2	2.25	0.48
1:E:102:GLU:O	1:E:105:LYS:HB3	2.13	0.48
1:E:185:ILE:HG23	1:E:345:LYS:C	2.38	0.48
1:A:180:GLU:HG3	1:G:104:LEU:CD1	2.44	0.48
1:B:245:ARG:NH1	1:B:304:ILE:HG22	2.29	0.48
1:C:111:GLY:CA	6:C:404:HOH:O	2.60	0.48
1:C:344:GLU:O	1:C:345:LYS:CB	2.61	0.48
1:D:313:VAL:HG22	1:D:327:LEU:HD23	1.94	0.48
1:E:314:TYR:HB3	1:E:328:ILE:HD11	1.96	0.48
1:E:331:PRO:HG3	1:F:140:PHE:CZ	2.48	0.48
1:B:225:LEU:O	1:B:228:THR:HB	2.14	0.48
1:D:182:ILE:HD12	1:D:197:LEU:CD2	2.44	0.48
1:D:196:VAL:C	1:D:198:LYS:H	2.21	0.48
1:E:212:MSE:HE1	1:E:260:LYS:HD3	1.94	0.48
1:E:334:PRO:C	1:E:335:GLU:HG3	2.38	0.48
1:F:117:SER:HB2	1:F:348:GLU:O	2.13	0.48
1:F:207:ASN:HA	1:F:243:HIS:ND1	2.28	0.48
1:F:258:GLN:NE2	1:F:258:GLN:CA	2.64	0.48
1:G:105:LYS:O	1:G:108:ALA:HB3	2.14	0.48
1:G:188:ASN:O	1:G:345:LYS:HG2	2.14	0.48
1:A:98:MSE:HG2	1:A:102:GLU:HB3	1.96	0.48
1:B:101:ASP:HB3	1:C:197:LEU:O	2.14	0.48
1:D:157:LEU:O	1:D:163:GLY:HA3	2.13	0.48
1:F:189:ARG:HG3	1:F:189:ARG:NH2	2.29	0.48
1:F:196:VAL:C	1:F:198:LYS:H	2.22	0.48
1:G:192:ASP:OD2	1:G:195:GLU:HB2	2.14	0.48
1:B:201:TYR:CD1	1:B:201:TYR:N	2.81	0.48
1:C:144:LYS:HG2	2:C:352:SO4:O4	2.14	0.48
1:C:195:GLU:HA	1:C:198:LYS:HD2	1.95	0.48
1:D:123:LEU:HD23	1:D:123:LEU:C	2.38	0.48
1:G:146:GLN:HE22	1:G:181:ARG:HE	1.62	0.48
1:A:303:HIS:ND1	1:A:303:HIS:C	2.72	0.47
1:D:201:TYR:CD1	1:D:201:TYR:N	2.82	0.47
1:E:243:HIS:O	1:E:247:GLU:HG3	2.13	0.47
1:G:121:ASP:HB3	1:G:126:GLY:O	2.14	0.47
1:G:196:VAL:C	1:G:198:LYS:N	2.70	0.47
1:G:331:PRO:O	1:G:332:HIS:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:SER:O	1:A:121:ASP:OD1	2.32	0.47
1:A:304:ILE:HG13	1:A:305:LEU:H	1.79	0.47
1:C:241:THR:OG1	1:C:283:ASN:ND2	2.47	0.47
1:C:316:ARG:NH1	1:C:337:GLU:OE2	2.43	0.47
1:F:251:ARG:C	1:F:253:ALA:N	2.72	0.47
1:G:211:GLN:HE21	1:G:264:HIS:HE1	1.62	0.47
1:B:333:LEU:HD12	1:B:333:LEU:N	2.29	0.47
1:D:211:GLN:HE21	1:D:264:HIS:CE1	2.33	0.47
1:D:241:THR:OG1	1:D:283:ASN:ND2	2.47	0.47
1:E:238:ASP:HA	1:E:239:SER:HA	1.74	0.47
1:F:147:LEU:HA	1:F:347:ILE:HD11	1.97	0.47
1:G:225:LEU:HD12	1:G:228:THR:HB	1.96	0.47
1:D:133:ILE:HD13	1:D:269:HIS:ND1	2.29	0.47
1:F:188:ASN:ND2	1:F:344:GLU:HG2	2.29	0.47
1:G:316:ARG:NH1	1:G:326:ARG:HH21	2.13	0.47
1:A:197:LEU:HD11	1:G:104:LEU:HD22	1.96	0.47
1:C:119:SER:H	1:C:349:ASP:CG	2.21	0.47
1:C:186:ALA:HB1	1:C:193:PRO:HA	1.96	0.47
1:F:274:LEU:HD12	1:F:275:TYR:CE2	2.49	0.47
1:A:243:HIS:O	1:A:247:GLU:HG3	2.14	0.47
1:A:274:LEU:HD12	1:A:275:TYR:CE2	2.49	0.47
1:B:118:LYS:HB2	1:B:349:ASP:CG	2.39	0.47
1:C:111:GLY:N	6:C:404:HOH:O	2.47	0.47
1:E:201:TYR:CD1	1:E:201:TYR:N	2.82	0.47
1:F:113:ILE:HD11	1:F:164:LEU:CD1	2.43	0.47
1:F:211:GLN:HE21	1:F:264:HIS:CE1	2.33	0.47
1:F:286:GLN:CD	1:F:286:GLN:N	2.72	0.47
1:A:76:ILE:HD13	1:A:76:ILE:N	2.30	0.47
1:A:115:THR:CB	1:A:120:LEU:HD23	2.44	0.47
1:A:201:TYR:N	1:A:201:TYR:CD1	2.83	0.47
1:A:225:LEU:O	1:A:228:THR:HB	2.15	0.47
1:B:183:ARG:HG2	1:B:183:ARG:HH11	1.80	0.47
1:B:188:ASN:OD1	1:B:344:GLU:HB3	2.14	0.47
1:D:139:GLU:CD	1:D:286:GLN:HG2	2.38	0.47
1:D:189:ARG:NE	1:D:345:LYS:HB3	2.28	0.47
1:E:123:LEU:HG	1:E:327:LEU:CD1	2.45	0.47
1:F:211:GLN:HE21	1:F:264:HIS:HE1	1.62	0.47
1:G:157:LEU:O	1:G:163:GLY:HA3	2.14	0.47
1:G:241:THR:OG1	1:G:283:ASN:ND2	2.48	0.47
1:G:251:ARG:HD3	1:G:252:GLY:N	2.29	0.47
1:A:251:ARG:HG3	1:A:251:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:PHE:HA	1:D:349:ASP:C	2.39	0.47
1:F:320:GLY:C	1:F:322:LYS:H	2.23	0.47
1:G:228:THR:CG2	1:G:229:ASP:N	2.78	0.47
1:A:228:THR:CG2	1:A:229:ASP:N	2.77	0.47
1:A:235:LEU:C	1:A:235:LEU:HD23	2.40	0.47
1:C:254:LEU:HD12	1:C:254:LEU:O	2.14	0.47
1:D:348:GLU:O	1:D:349:ASP:HB2	2.14	0.47
1:E:333:LEU:HD12	1:E:334:PRO:HD2	1.97	0.47
1:F:190:GLY:C	1:F:191:LEU:HD23	2.40	0.47
1:F:241:THR:OG1	1:F:283:ASN:ND2	2.47	0.47
1:A:230:ARG:NH1	1:A:230:ARG:HG2	2.30	0.47
1:A:249:ILE:HD12	1:A:249:ILE:H	1.73	0.47
1:C:123:LEU:HD21	1:C:336:GLY:O	2.14	0.46
1:C:328:ILE:O	1:C:329:ASP:HB3	2.15	0.46
1:E:213:LEU:O	1:E:217:GLN:HG3	2.14	0.46
1:E:327:LEU:O	1:E:328:ILE:HD12	2.15	0.46
1:F:218:ALA:O	1:F:219:GLU:C	2.58	0.46
1:A:137:PHE:CZ	1:A:314:TYR:HB2	2.49	0.46
1:D:170:TRP:CE3	1:D:236:ILE:HD12	2.50	0.46
1:F:142:SER:C	1:F:323:ARG:HD2	2.40	0.46
1:F:243:HIS:O	1:F:247:GLU:HG3	2.14	0.46
1:C:192:ASP:OD2	1:C:195:GLU:HB2	2.15	0.46
1:D:97:PHE:HE2	1:E:171:ILE:CD1	2.27	0.46
1:D:146:GLN:HE22	1:D:181:ARG:HE	1.63	0.46
1:E:322:LYS:HZ2	1:E:341:SER:HB3	1.80	0.46
1:E:331:PRO:CG	1:F:140:PHE:HZ	2.29	0.46
1:F:104:LEU:HB2	1:G:179:PRO:HB2	1.96	0.46
1:F:171:ILE:HD12	1:F:214:LEU:HB3	1.97	0.46
1:F:219:GLU:O	1:F:223:LYS:HG3	2.15	0.46
1:C:187:GLN:CB	1:C:193:PRO:HD3	2.44	0.46
1:C:201:TYR:CD1	1:C:201:TYR:N	2.83	0.46
1:D:304:ILE:HG12	1:D:305:LEU:N	2.30	0.46
1:E:219:GLU:CD	1:E:270:ARG:HH22	2.20	0.46
1:A:104:LEU:HD12	1:B:180:GLU:HG3	1.98	0.46
1:F:156:GLN:OE1	1:F:199:HIS:HB2	2.15	0.46
1:G:183:ARG:HH22	1:G:194:ASP:CG	2.23	0.46
1:G:192:ASP:HA	1:G:193:PRO:HD2	1.74	0.46
1:C:104:LEU:HD22	1:C:104:LEU:C	2.39	0.46
1:C:348:GLU:HG2	1:C:349:ASP:N	2.30	0.46
1:D:332:HIS:CE1	1:E:178:ARG:NE	2.78	0.46
1:A:124:LEU:HD12	1:A:127:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:NE	1:B:101:ASP:OD2	2.48	0.46
1:B:166:GLY:HA3	1:B:233:LYS:HG3	1.98	0.46
1:C:219:GLU:CD	1:C:270:ARG:HH22	2.23	0.46
1:C:274:LEU:HD12	1:C:275:TYR:CE2	2.51	0.46
1:G:327:LEU:N	1:G:327:LEU:CD1	2.79	0.46
1:G:329:ASP:HB3	1:G:330:ALA:H	1.52	0.46
1:A:158:PRO:HB3	1:A:160:GLU:OE1	2.16	0.46
1:E:332:HIS:O	1:E:333:LEU:CB	2.63	0.46
1:A:80:THR:O	1:A:84:ILE:HG12	2.15	0.46
1:B:187:GLN:HG3	1:B:188:ASN:H	1.79	0.46
1:C:316:ARG:HG2	1:C:324:ILE:HG23	1.98	0.46
1:D:187:GLN:CD	1:D:193:PRO:HG3	2.40	0.46
1:D:187:GLN:NE2	1:D:193:PRO:HG3	2.31	0.46
1:D:313:VAL:HG22	1:D:327:LEU:CD2	2.46	0.46
1:D:323:ARG:HD2	1:D:323:ARG:N	2.31	0.46
1:E:237:VAL:HB	1:E:281:VAL:HG12	1.98	0.46
1:G:120:LEU:CD2	1:G:124:LEU:HD12	2.45	0.46
1:A:189:ARG:NH2	1:A:345:LYS:O	2.49	0.46
1:B:189:ARG:NE	1:B:345:LYS:HB3	2.30	0.46
1:C:119:SER:O	1:C:122:LYS:HB3	2.15	0.46
1:D:186:ALA:O	1:D:188:ASN:N	2.40	0.46
1:E:286:GLN:H	1:E:303:HIS:HE1	1.56	0.46
1:G:120:LEU:O	1:G:121:ASP:C	2.59	0.46
1:G:140:PHE:HB2	1:G:284:GLN:OE1	2.16	0.46
1:B:137:PHE:HZ	1:B:328:ILE:HG12	1.82	0.45
1:D:186:ALA:C	1:D:188:ASN:H	2.24	0.45
1:D:207:ASN:CA	1:D:243:HIS:ND1	2.79	0.45
1:D:221:LYS:O	1:D:225:LEU:HD13	2.16	0.45
1:F:118:LYS:O	1:F:122:LYS:HG3	2.16	0.45
1:A:221:LYS:HG3	1:A:225:LEU:CD1	2.41	0.45
1:B:323:ARG:HE	1:B:342:ILE:CG1	2.26	0.45
1:E:133:ILE:HD11	1:E:269:HIS:HA	1.99	0.45
1:E:211:GLN:HE21	1:E:264:HIS:CE1	2.33	0.45
1:E:230:ARG:HH11	1:E:230:ARG:CB	2.28	0.45
1:E:329:ASP:CG	1:E:330:ALA:N	2.74	0.45
1:A:146:GLN:HE22	1:A:181:ARG:NE	2.14	0.45
1:B:285:VAL:HG13	1:B:285:VAL:O	2.16	0.45
1:D:326:ARG:NH1	1:D:337:GLU:OE2	2.49	0.45
1:G:122:LYS:C	1:G:124:LEU:N	2.74	0.45
1:G:243:HIS:O	1:G:247:GLU:HG3	2.16	0.45
1:B:187:GLN:C	1:B:189:ARG:N	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:VAL:HB	1:C:281:VAL:HG12	1.98	0.45
1:C:322:LYS:HG2	1:C:341:SER:HB3	1.98	0.45
1:D:243:HIS:O	1:D:247:GLU:HG3	2.16	0.45
1:F:157:LEU:HD13	1:F:161:GLU:HB3	1.98	0.45
1:G:303:HIS:CG	1:G:304:ILE:N	2.84	0.45
1:A:77:SER:OG	1:A:80:THR:HG23	2.17	0.45
1:A:99:ARG:O	1:A:102:GLU:N	2.49	0.45
1:A:158:PRO:HA	1:A:159:PRO:HD3	1.86	0.45
1:A:344:GLU:CD	1:A:344:GLU:N	2.72	0.45
1:C:158:PRO:HA	1:C:159:PRO:HD3	1.85	0.45
1:E:158:PRO:HD2	1:E:161:GLU:HG3	1.98	0.45
1:A:156:GLN:OE1	1:A:199:HIS:HB2	2.16	0.45
1:A:160:GLU:OE2	1:A:160:GLU:N	2.49	0.45
1:A:258:GLN:CG	1:B:249:ILE:HD11	2.47	0.45
1:C:269:HIS:HB3	1:D:206:PHE:CE2	2.52	0.45
1:G:122:LYS:C	1:G:124:LEU:H	2.25	0.45
1:G:305:LEU:HG	1:G:306:ALA:N	2.31	0.45
1:G:324:ILE:C	1:G:324:ILE:CD1	2.83	0.45
1:A:43:VAL:HG23	1:A:84:ILE:HD12	1.98	0.45
1:B:182:ILE:HD13	1:B:200:ILE:CD1	2.47	0.45
1:B:185:ILE:HA	6:B:386:HOH:O	2.16	0.45
1:D:307:HIS:ND1	1:D:308:SER:N	2.65	0.45
1:E:211:GLN:HE21	1:E:264:HIS:HE1	1.64	0.45
1:F:245:ARG:HB3	1:F:304:ILE:CD1	2.41	0.45
1:G:344:GLU:O	1:G:345:LYS:CB	2.61	0.45
1:A:184:GLU:O	1:A:185:ILE:C	2.60	0.45
1:C:159:PRO:HA	1:C:163:GLY:O	2.17	0.45
1:D:169:ILE:HG13	1:D:222:ILE:CD1	2.33	0.45
1:D:185:ILE:O	1:D:189:ARG:HG2	2.17	0.45
1:E:333:LEU:CD1	1:E:334:PRO:HD2	2.47	0.45
1:G:274:LEU:HD12	1:G:275:TYR:CE2	2.52	0.45
1:A:251:ARG:HE	1:B:251:ARG:HH22	1.64	0.45
1:A:265:LEU:HD21	1:A:306:ALA:HA	1.98	0.45
1:D:211:GLN:HE21	1:D:264:HIS:HE1	1.65	0.45
1:D:305:LEU:HB2	1:D:312:ARG:HH21	1.82	0.45
1:E:117:SER:HB3	1:E:347:ILE:HG22	1.98	0.45
1:E:329:ASP:CG	1:E:331:PRO:HD2	2.42	0.45
1:F:170:TRP:CE3	1:F:236:ILE:HD12	2.52	0.45
1:A:146:GLN:HG2	6:A:421:HOH:O	2.17	0.45
1:A:324:ILE:HD12	1:A:325:ALA:N	2.32	0.45
1:B:115:THR:HA	1:B:151:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:PRO:HA	1:D:159:PRO:HD3	1.81	0.45
1:E:164:LEU:O	1:E:165:ASN:C	2.59	0.45
1:G:106:LYS:C	1:G:108:ALA:N	2.75	0.45
1:A:49:GLU:OE2	1:A:49:GLU:HA	2.15	0.44
1:A:91:ALA:O	1:A:92:ALA:C	2.60	0.44
1:A:258:GLN:HG3	1:B:249:ILE:HD11	1.99	0.44
1:C:179:PRO:O	1:C:180:GLU:C	2.60	0.44
1:C:181:ARG:CZ	1:C:185:ILE:HD11	2.47	0.44
1:C:196:VAL:C	1:C:198:LYS:N	2.74	0.44
1:F:142:SER:O	1:F:315:LEU:HD13	2.17	0.44
1:F:218:ALA:O	1:F:221:LYS:N	2.50	0.44
1:C:224:GLU:N	1:C:224:GLU:OE1	2.50	0.44
1:D:166:GLY:HA3	1:D:233:LYS:HG3	1.99	0.44
1:D:328:ILE:O	1:D:329:ASP:HB3	2.16	0.44
1:F:140:PHE:HB2	1:F:284:GLN:OE1	2.17	0.44
1:F:146:GLN:NE2	1:F:181:ARG:HE	2.15	0.44
1:F:222:ILE:N	1:F:222:ILE:HD12	2.32	0.44
1:G:238:ASP:HA	1:G:239:SER:HA	1.70	0.44
1:B:101:ASP:CG	1:B:102:GLU:H	2.24	0.44
1:B:179:PRO:HD2	1:B:180:GLU:OE1	2.16	0.44
1:B:221:LYS:O	1:B:222:ILE:C	2.58	0.44
1:D:115:THR:O	1:D:150:THR:HG21	2.17	0.44
1:E:101:ASP:OD1	1:E:102:GLU:N	2.50	0.44
1:F:192:ASP:O	1:F:195:GLU:N	2.49	0.44
1:A:113:ILE:HD12	1:A:164:LEU:HG	1.98	0.44
1:A:286:GLN:NE2	1:A:286:GLN:CA	2.80	0.44
1:B:123:LEU:HA	1:B:334:PRO:HG3	1.98	0.44
1:B:183:ARG:HG2	1:B:183:ARG:NH1	2.33	0.44
1:C:181:ARG:NH2	1:C:181:ARG:HG3	2.32	0.44
1:E:250:GLY:O	1:E:253:ALA:HB3	2.16	0.44
1:F:207:ASN:CA	1:F:243:HIS:ND1	2.81	0.44
1:G:186:ALA:C	1:G:188:ASN:H	2.25	0.44
1:G:285:VAL:O	1:G:285:VAL:HG13	2.18	0.44
1:A:243:HIS:HD2	1:G:307:HIS:HE1	1.64	0.44
1:C:328:ILE:O	1:C:329:ASP:CB	2.65	0.44
1:G:140:PHE:C	1:G:140:PHE:CD1	2.95	0.44
1:G:192:ASP:O	1:G:194:ASP:N	2.50	0.44
1:B:181:ARG:HD2	1:B:181:ARG:O	2.16	0.44
1:B:210:HIS:O	1:B:213:LEU:HB3	2.18	0.44
1:B:223:LYS:O	1:B:224:GLU:C	2.60	0.44
1:E:241:THR:OG1	1:E:283:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HH21	1:B:178:ARG:NE	2.16	0.44
1:A:245:ARG:NH1	1:A:304:ILE:HG22	2.32	0.44
1:B:185:ILE:O	1:B:189:ARG:HB2	2.18	0.44
1:B:254:LEU:H	3:B:359:IMD:C4	2.31	0.44
1:C:324:ILE:HD11	1:C:337:GLU:CD	2.43	0.44
1:F:164:LEU:O	1:F:165:ASN:C	2.59	0.44
1:G:99:ARG:CB	1:G:99:ARG:HH11	2.31	0.44
1:A:320:GLY:HA2	3:A:361:IMD:HN3	1.82	0.44
1:A:324:ILE:HD12	1:A:324:ILE:C	2.42	0.44
1:A:332:HIS:O	1:A:333:LEU:CB	2.59	0.44
1:B:219:GLU:O	1:B:220:ASP:C	2.59	0.44
1:D:195:GLU:HA	1:D:198:LYS:HD2	1.99	0.44
1:F:222:ILE:O	1:F:226:LEU:HB2	2.17	0.44
1:B:212:MSE:O	1:B:216:GLN:HG3	2.17	0.44
1:B:251:ARG:HG2	1:B:251:ARG:HH21	1.83	0.44
1:E:113:ILE:O	1:E:127:GLY:HA3	2.18	0.44
1:A:97:PHE:HE2	1:B:171:ILE:CD1	2.31	0.43
1:A:201:TYR:CZ	1:A:225:LEU:HD21	2.53	0.43
1:B:187:GLN:CG	1:B:188:ASN:N	2.80	0.43
1:C:185:ILE:HG23	1:C:345:LYS:C	2.43	0.43
1:C:186:ALA:CB	1:C:193:PRO:HA	2.48	0.43
1:C:285:VAL:O	1:C:285:VAL:HG13	2.18	0.43
1:F:123:LEU:HD22	1:F:338:ALA:CB	2.48	0.43
1:A:133:ILE:HD13	1:A:269:HIS:ND1	2.33	0.43
1:B:340:PHE:CD1	1:B:347:ILE:HG23	2.53	0.43
1:D:329:ASP:HB2	1:D:331:PRO:HD2	2.00	0.43
1:G:182:ILE:CG2	1:G:196:VAL:HG11	2.48	0.43
1:G:257:ARG:O	1:G:261:LEU:HB2	2.18	0.43
1:A:251:ARG:HG2	1:B:251:ARG:CG	2.48	0.43
1:B:170:TRP:CE3	1:B:236:ILE:HD12	2.54	0.43
1:C:140:PHE:HB2	1:C:284:GLN:OE1	2.18	0.43
1:C:265:LEU:HD21	1:C:306:ALA:HB1	1.99	0.43
1:E:166:GLY:HA3	1:E:233:LYS:HG3	1.99	0.43
1:E:248:TYR:C	1:E:249:ILE:HD12	2.42	0.43
1:E:331:PRO:HG3	1:F:140:PHE:HZ	1.83	0.43
1:F:117:SER:O	1:F:118:LYS:C	2.61	0.43
1:A:147:LEU:HA	1:A:347:ILE:CD1	2.48	0.43
1:A:164:LEU:HD12	1:A:233:LYS:HD3	2.00	0.43
1:D:170:TRP:HB3	1:D:202:VAL:HG13	2.00	0.43
1:D:323:ARG:NH1	1:D:323:ARG:HG3	2.34	0.43
1:F:104:LEU:HB2	1:G:179:PRO:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:THR:HA	1:F:151:LEU:CD1	2.48	0.43
1:A:158:PRO:O	1:A:161:GLU:HB2	2.18	0.43
1:A:201:TYR:CD2	1:A:221:LYS:HD3	2.53	0.43
1:C:251:ARG:CZ	1:D:251:ARG:HA	2.47	0.43
1:D:186:ALA:C	1:D:188:ASN:N	2.76	0.43
1:F:129:GLU:HG3	6:F:396:HOH:O	2.19	0.43
1:F:140:PHE:CD1	1:F:140:PHE:C	2.96	0.43
1:F:324:ILE:C	1:F:324:ILE:CD1	2.91	0.43
1:C:224:GLU:O	1:C:226:LEU:N	2.51	0.43
1:F:240:LEU:HD21	1:F:265:LEU:HD11	2.00	0.43
1:F:269:HIS:NE2	1:F:308:SER:HB3	2.34	0.43
1:G:115:THR:O	1:G:150:THR:HG21	2.19	0.43
1:A:178:ARG:C	1:A:180:GLU:N	2.76	0.43
1:A:248:TYR:C	1:A:249:ILE:HD12	2.42	0.43
1:A:323:ARG:HG3	1:A:323:ARG:HH11	1.83	0.43
1:B:118:LYS:N	1:B:349:ASP:HB2	2.27	0.43
1:B:219:GLU:OE1	1:B:270:ARG:NH2	2.52	0.43
1:C:263:LYS:HD3	1:C:267:ASP:OD2	2.17	0.43
1:D:115:THR:HA	1:D:151:LEU:CD1	2.49	0.43
1:D:193:PRO:HA	1:D:196:VAL:HG23	2.00	0.43
1:E:269:HIS:HB3	1:F:206:PHE:CD2	2.53	0.43
1:F:344:GLU:CD	1:F:344:GLU:N	2.74	0.43
1:A:168:VAL:HG22	1:A:234:LEU:HB3	1.99	0.43
1:B:147:LEU:HD22	1:B:151:LEU:HD22	2.01	0.43
1:B:238:ASP:HA	1:B:239:SER:HA	1.72	0.43
1:C:101:ASP:O	1:C:104:LEU:HB3	2.18	0.43
1:C:124:LEU:HA	1:C:333:LEU:HD23	2.00	0.43
1:D:97:PHE:HE2	1:E:171:ILE:HD13	1.82	0.43
1:D:328:ILE:HD12	1:D:328:ILE:N	2.33	0.43
1:E:113:ILE:N	1:E:113:ILE:HD13	2.33	0.43
1:G:324:ILE:HD11	1:G:337:GLU:HB3	2.01	0.43
1:D:237:VAL:HB	1:D:281:VAL:HG12	2.01	0.43
1:F:98:MSE:O	1:G:201:TYR:HA	2.19	0.43
1:A:98:MSE:CG	1:A:102:GLU:HB3	2.48	0.43
1:B:128:ILE:O	1:B:128:ILE:HG13	2.17	0.43
1:B:243:HIS:O	1:B:247:GLU:HG3	2.19	0.43
1:D:147:LEU:HD22	1:D:151:LEU:HD22	2.01	0.43
1:A:171:ILE:CD1	1:G:97:PHE:CE1	3.00	0.42
1:B:251:ARG:C	1:B:253:ALA:N	2.76	0.42
1:B:316:ARG:HG2	1:B:324:ILE:HG23	2.01	0.42
1:C:265:LEU:HD21	1:C:306:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:ILE:HA	1:E:338:ALA:O	2.19	0.42
1:F:305:LEU:N	1:F:305:LEU:HD23	2.33	0.42
1:B:207:ASN:HB2	1:B:247:GLU:OE1	2.19	0.42
1:F:218:ALA:O	1:F:222:ILE:HD13	2.19	0.42
1:B:274:LEU:HD13	1:B:274:LEU:O	2.19	0.42
1:B:283:ASN:C	1:B:283:ASN:HD22	2.26	0.42
1:D:140:PHE:HB2	1:D:284:GLN:OE1	2.19	0.42
1:D:274:LEU:HD12	1:D:275:TYR:CE2	2.54	0.42
1:F:100:ALA:HB2	1:G:200:ILE:HB	2.00	0.42
1:G:117:SER:O	1:G:118:LYS:C	2.60	0.42
1:B:223:LYS:O	1:B:226:LEU:CB	2.67	0.42
1:C:222:ILE:CG2	1:C:277:ILE:HD11	2.49	0.42
1:D:146:GLN:HE21	1:D:146:GLN:CA	2.23	0.42
1:D:324:ILE:HB	1:D:339:VAL:HG22	1.99	0.42
1:G:182:ILE:O	1:G:183:ARG:C	2.62	0.42
1:G:340:PHE:CD1	1:G:347:ILE:HG23	2.54	0.42
1:A:105:LYS:HE3	1:A:105:LYS:HA	2.02	0.42
1:B:228:THR:CG2	1:B:229:ASP:N	2.82	0.42
1:C:221:LYS:O	1:C:225:LEU:HD23	2.19	0.42
1:C:340:PHE:CD1	1:C:347:ILE:HG23	2.54	0.42
1:B:105:LYS:NZ	1:B:109:THR:HG21	2.34	0.42
1:B:147:LEU:HA	1:B:347:ILE:CD1	2.49	0.42
1:B:223:LYS:O	1:B:226:LEU:HB3	2.20	0.42
1:C:164:LEU:O	1:C:165:ASN:C	2.63	0.42
1:D:112:ARG:HD3	1:D:125:GLY:O	2.20	0.42
1:F:192:ASP:O	1:F:193:PRO:C	2.61	0.42
1:F:227:ASN:H	1:F:227:ASN:ND2	2.18	0.42
1:F:251:ARG:N	1:F:251:ARG:CD	2.79	0.42
1:A:333:LEU:HB3	1:A:334:PRO:HD2	2.02	0.42
1:B:188:ASN:HD22	1:B:188:ASN:HA	1.59	0.42
1:D:160:GLU:CD	1:D:160:GLU:N	2.73	0.42
1:E:170:TRP:CE3	1:E:236:ILE:HD12	2.55	0.42
1:E:331:PRO:HB3	1:F:140:PHE:HZ	1.85	0.42
1:F:147:LEU:HG	1:F:347:ILE:CD1	2.50	0.42
1:A:97:PHE:CD1	1:A:97:PHE:N	2.88	0.42
1:C:316:ARG:HG2	1:C:324:ILE:CG2	2.50	0.42
1:D:265:LEU:HA	1:D:265:LEU:HD12	1.80	0.42
1:E:140:PHE:CD1	1:E:140:PHE:C	2.96	0.42
1:A:66:SER:OG	1:A:69:GLU:HG3	2.20	0.42
1:A:225:LEU:N	1:A:225:LEU:CD1	2.83	0.42
1:A:323:ARG:NH1	1:A:323:ARG:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ALA:HB2	1:B:196:VAL:HG21	2.01	0.42
1:E:123:LEU:CG	1:E:327:LEU:HD13	2.50	0.42
1:E:147:LEU:HA	1:E:347:ILE:CD1	2.50	0.42
1:F:330:ALA:N	1:F:331:PRO:CD	2.82	0.42
1:B:323:ARG:NH2	1:B:323:ARG:HG3	2.32	0.42
1:E:115:THR:HA	1:E:151:LEU:CD1	2.50	0.42
1:E:308:SER:O	1:E:309:ALA:C	2.62	0.42
1:A:76:ILE:HD13	1:A:76:ILE:H	1.85	0.41
1:B:112:ARG:H	1:B:164:LEU:HD21	1.85	0.41
1:B:328:ILE:H	1:B:328:ILE:CD1	2.26	0.41
1:D:225:LEU:H	1:D:225:LEU:CD1	2.33	0.41
1:D:238:ASP:HA	1:D:239:SER:HA	1.68	0.41
1:E:103:TYR:C	1:E:105:LYS:N	2.74	0.41
1:A:104:LEU:HD23	1:A:105:LYS:HD2	2.02	0.41
1:A:171:ILE:HD11	1:G:97:PHE:CE1	2.54	0.41
1:A:317:LYS:HG3	1:A:323:ARG:CZ	2.45	0.41
1:B:147:LEU:HA	1:B:347:ILE:HD11	2.01	0.41
1:B:171:ILE:HD12	1:B:214:LEU:HB3	2.02	0.41
1:C:179:PRO:HB2	1:C:197:LEU:HD11	2.01	0.41
1:C:243:HIS:O	1:C:247:GLU:HG3	2.21	0.41
1:C:285:VAL:O	1:C:286:GLN:HB2	2.20	0.41
1:D:185:ILE:HG23	1:D:345:LYS:C	2.45	0.41
1:E:329:ASP:OD2	1:E:329:ASP:C	2.62	0.41
1:E:332:HIS:O	1:E:333:LEU:HB2	2.19	0.41
1:F:218:ALA:C	1:F:222:ILE:HD13	2.45	0.41
1:G:189:ARG:HE	1:G:345:LYS:HB3	1.85	0.41
1:G:333:LEU:CB	1:G:334:PRO:HD2	2.50	0.41
1:C:100:ALA:HB2	1:D:200:ILE:HB	2.03	0.41
1:C:115:THR:HA	1:C:151:LEU:CD1	2.50	0.41
1:D:175:ASN:H	1:D:204:ARG:NH1	2.18	0.41
1:E:119:SER:CB	1:E:349:ASP:OD1	2.67	0.41
1:E:229:ASP:O	1:E:231:PRO:HD3	2.20	0.41
1:F:146:GLN:HE21	1:F:146:GLN:CA	2.21	0.41
1:F:181:ARG:O	1:F:185:ILE:HG13	2.20	0.41
1:A:62:ILE:HG23	1:A:70:LEU:HD11	2.02	0.41
1:A:230:ARG:HG2	1:A:230:ARG:HH11	1.86	0.41
1:B:105:LYS:O	1:B:108:ALA:HB3	2.21	0.41
1:B:113:ILE:HD13	1:B:113:ILE:N	2.34	0.41
1:B:344:GLU:C	1:B:346:GLY:H	2.27	0.41
1:E:113:ILE:HD11	1:E:164:LEU:CD1	2.51	0.41
1:A:37:ILE:HD13	6:A:430:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HD23	1:A:147:LEU:O	2.21	0.41
1:A:258:GLN:CG	1:B:249:ILE:CD1	2.96	0.41
1:D:207:ASN:N	1:D:243:HIS:CE1	2.89	0.41
1:E:213:LEU:HD13	1:E:217:GLN:OE1	2.20	0.41
1:F:113:ILE:CD1	1:F:164:LEU:CD1	2.98	0.41
1:G:305:LEU:HG	1:G:307:HIS:N	2.34	0.41
1:G:329:ASP:O	1:G:330:ALA:CB	2.68	0.41
1:G:344:GLU:CD	1:G:344:GLU:N	2.74	0.41
1:D:323:ARG:HG3	1:D:323:ARG:HH11	1.85	0.41
1:E:157:LEU:O	1:E:163:GLY:HA3	2.20	0.41
1:F:170:TRP:HB3	1:F:202:VAL:HG13	2.02	0.41
1:A:348:GLU:O	1:A:349:ASP:CB	2.69	0.41
1:B:221:LYS:HE2	1:B:225:LEU:CD2	2.51	0.41
1:E:147:LEU:HD22	1:E:151:LEU:HD22	2.02	0.41
1:F:147:LEU:CA	1:F:347:ILE:HD11	2.50	0.41
1:F:258:GLN:HG3	1:G:249:ILE:HD12	2.01	0.41
1:G:147:LEU:HD22	1:G:151:LEU:HD22	2.02	0.41
1:G:182:ILE:O	1:G:185:ILE:HG23	2.20	0.41
1:A:142:SER:HB2	1:A:315:LEU:HD12	2.02	0.41
1:A:209:ASN:O	1:A:213:LEU:HB2	2.20	0.41
1:C:170:TRP:HB3	1:C:202:VAL:HG13	1.98	0.41
1:E:322:LYS:HZ3	1:E:341:SER:HB3	1.85	0.41
1:F:238:ASP:HA	1:F:239:SER:HA	1.73	0.41
1:A:153:VAL:O	1:A:154:MSE:C	2.64	0.41
1:B:140:PHE:CD1	1:B:140:PHE:C	2.98	0.41
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.92	0.41
1:B:254:LEU:HD21	1:C:249:ILE:CG2	2.51	0.41
1:C:131:GLN:HA	1:C:272:ALA:O	2.21	0.41
1:C:265:LEU:HD21	1:C:306:ALA:HA	2.03	0.41
1:D:97:PHE:CD2	1:E:203:ALA:HB2	2.55	0.41
1:D:154:MSE:O	1:D:157:LEU:HG	2.19	0.41
1:D:187:GLN:O	1:D:187:GLN:HG3	2.21	0.41
1:F:229:ASP:C	1:F:231:PRO:HD3	2.45	0.41
1:F:265:LEU:HD12	1:F:265:LEU:HA	1.89	0.41
1:F:316:ARG:HG2	1:F:324:ILE:CG2	2.51	0.41
1:G:116:GLY:O	1:G:348:GLU:HA	2.21	0.41
1:G:156:GLN:HE21	1:G:196:VAL:HG13	1.81	0.41
1:G:158:PRO:HA	1:G:159:PRO:HD3	1.87	0.41
1:G:237:VAL:HB	1:G:281:VAL:HG12	2.02	0.41
1:G:314:TYR:CB	1:G:328:ILE:HD11	2.50	0.41
1:B:348:GLU:OE2	1:B:348:GLU:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:GLN:HB3	1:C:193:PRO:CG	2.50	0.41
1:C:286:GLN:NE2	1:C:286:GLN:CA	2.82	0.41
1:D:140:PHE:CD1	1:D:140:PHE:C	2.98	0.41
1:D:344:GLU:CD	1:D:344:GLU:N	2.76	0.41
1:E:221:LYS:HD2	1:E:221:LYS:HA	1.86	0.41
1:G:120:LEU:HD22	1:G:124:LEU:HD12	2.03	0.41
1:G:122:LYS:O	1:G:124:LEU:N	2.53	0.41
1:B:324:ILE:HD12	1:B:338:ALA:C	2.45	0.40
1:D:100:ALA:HB3	1:E:197:LEU:O	2.21	0.40
1:D:308:SER:HB3	1:D:309:ALA:H	1.72	0.40
1:D:323:ARG:HD3	1:D:342:ILE:HD11	2.04	0.40
1:G:184:GLU:O	1:G:186:ALA:N	2.54	0.40
1:A:170:TRP:CE3	1:A:236:ILE:HD12	2.56	0.40
1:C:251:ARG:HH21	1:D:251:ARG:CA	2.25	0.40
1:D:136:VAL:O	1:D:136:VAL:HG13	2.21	0.40
1:D:158:PRO:HD2	1:D:161:GLU:OE2	2.21	0.40
1:D:188:ASN:CG	1:D:344:GLU:HB3	2.44	0.40
1:F:192:ASP:HA	1:F:193:PRO:HD2	1.96	0.40
1:F:219:GLU:O	1:F:219:GLU:HG3	2.20	0.40
1:G:166:GLY:HA3	1:G:233:LYS:HG3	2.02	0.40
1:A:136:VAL:O	1:A:136:VAL:HG13	2.21	0.40
1:A:183:ARG:HE	1:A:193:PRO:HB2	1.87	0.40
1:D:195:GLU:O	1:D:198:LYS:HB2	2.22	0.40
1:E:205:ALA:O	1:E:243:HIS:HE1	2.03	0.40
1:G:344:GLU:C	1:G:346:GLY:H	2.29	0.40
1:D:147:LEU:HA	1:D:347:ILE:CD1	2.52	0.40
1:D:147:LEU:HG	1:D:347:ILE:CD1	2.52	0.40
1:E:140:PHE:HB2	1:E:284:GLN:OE1	2.21	0.40
1:G:212:MSE:HE1	1:G:260:LYS:HD3	2.03	0.40
1:G:261:LEU:HD13	1:G:304:ILE:HD11	2.04	0.40
1:A:60:GLU:HA	1:A:63:ALA:HB3	2.03	0.40
1:A:179:PRO:HD2	1:A:180:GLU:OE1	2.21	0.40
1:E:156:GLN:HE21	1:E:196:VAL:HG13	1.79	0.40
1:E:318:GLY:O	1:E:319:LYS:O	2.39	0.40
1:F:157:LEU:HD13	1:F:161:GLU:HB2	2.03	0.40
1:F:207:ASN:N	1:F:243:HIS:CE1	2.90	0.40
1:G:225:LEU:HD12	1:G:225:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	296/349 (85%)	265 (90%)	20 (7%)	11 (4%)	2	5
1	B	235/349 (67%)	203 (86%)	25 (11%)	7 (3%)	3	8
1	C	235/349 (67%)	199 (85%)	25 (11%)	11 (5%)	2	3
1	D	235/349 (67%)	199 (85%)	26 (11%)	10 (4%)	2	4
1	E	235/349 (67%)	212 (90%)	15 (6%)	8 (3%)	3	6
1	F	235/349 (67%)	207 (88%)	23 (10%)	5 (2%)	5	13
1	G	234/349 (67%)	187 (80%)	31 (13%)	16 (7%)	1	1
All	All	1705/2443 (70%)	1472 (86%)	165 (10%)	68 (4%)	2	4

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
1	A	319	LYS
1	A	334	PRO
1	B	329	ASP
1	B	330	ALA
1	C	329	ASP
1	C	330	ALA
1	D	191	LEU
1	D	319	LYS
1	D	329	ASP
1	D	330	ALA
1	E	303	HIS
1	E	319	LYS
1	E	329	ASP
1	E	330	ALA
1	E	334	PRO
1	F	319	LYS
1	G	184	GLU

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Mol	Chain	Res	Type
1	G	191	LEU
1	G	197	LEU
1	G	225	LEU
1	G	330	ALA
1	G	333	LEU
1	G	334	PRO
1	A	184	GLU
1	A	185	ILE
1	B	252	GLY
1	B	319	LYS
1	C	197	LEU
1	C	225	LEU
1	C	253	ALA
1	D	250	GLY
1	D	308	SER
1	E	332	HIS
1	F	219	GLU
1	G	185	ILE
1	G	224	GLU
1	G	329	ASP
1	A	303	HIS
1	A	329	ASP
1	B	188	ASN
1	C	186	ALA
1	C	224	GLU
1	C	319	LYS
1	D	184	GLU
1	D	186	ALA
1	F	197	LEU
1	F	332	HIS
1	G	193	PRO
1	G	223	LYS
1	G	326	ARG
1	C	188	ASN
1	D	197	LEU
1	G	123	LEU
1	D	164	LEU
1	E	253	ALA
1	E	333	LEU
1	G	122	LYS
1	G	307	HIS
1	A	37	ILE

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Mol	Chain	Res	Type
1	A	330	ALA
1	A	333	LEU
1	C	334	PRO
1	A	192	ASP
1	B	333	LEU
1	B	334	PRO
1	C	333	LEU
1	F	334	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/279 (87%)	217 (90%)	25 (10%)	7	14
1	B	199/279 (71%)	178 (89%)	21 (11%)	6	13
1	C	199/279 (71%)	177 (89%)	22 (11%)	6	12
1	D	199/279 (71%)	174 (87%)	25 (13%)	4	8
1	E	199/279 (71%)	180 (90%)	19 (10%)	8	17
1	F	199/279 (71%)	179 (90%)	20 (10%)	7	15
1	G	199/279 (71%)	178 (89%)	21 (11%)	6	13
All	All	1436/1953 (74%)	1283 (89%)	153 (11%)	6	13

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	37	ILE
1	A	41	PRO
1	A	64	VAL
1	A	76	ILE
1	A	89	ARG
1	A	93	ASN
1	A	94	LEU
1	A	102	GLU

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Mol	Chain	Res	Type
1	A	104	LEU
1	A	107	ARG
1	A	112	ARG
1	A	113	ILE
1	A	129	GLU
1	A	147	LEU
1	A	151	LEU
1	A	160	GLU
1	A	202	VAL
1	A	249	ILE
1	A	254	LEU
1	A	265	LEU
1	A	274	LEU
1	A	305	LEU
1	A	324	ILE
1	A	342	ILE
1	B	120	LEU
1	B	129	GLU
1	B	151	LEU
1	B	160	GLU
1	B	182	ILE
1	B	196	VAL
1	B	202	VAL
1	B	221	LYS
1	B	225	LEU
1	B	229	ASP
1	B	249	ILE
1	B	251	ARG
1	B	261	LEU
1	B	265	LEU
1	B	274	LEU
1	B	304	ILE
1	B	305	LEU
1	B	328	ILE
1	B	332	HIS
1	B	342	ILE
1	B	348	GLU
1	C	97	PHE
1	C	99	ARG
1	C	104	LEU
1	C	107	ARG
1	C	120	LEU

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Mol	Chain	Res	Type
1	C	129	GLU
1	C	147	LEU
1	C	151	LEU
1	C	191	LEU
1	C	197	LEU
1	C	202	VAL
1	C	216	GLN
1	C	221	LYS
1	C	224	GLU
1	C	257	ARG
1	C	261	LEU
1	C	265	LEU
1	C	274	LEU
1	C	316	ARG
1	C	327	LEU
1	C	342	ILE
1	C	348	GLU
1	D	105	LYS
1	D	120	LEU
1	D	129	GLU
1	D	147	LEU
1	D	151	LEU
1	D	196	VAL
1	D	202	VAL
1	D	204	ARG
1	D	213	LEU
1	D	216	GLN
1	D	221	LYS
1	D	222	ILE
1	D	223	LYS
1	D	224	GLU
1	D	259	GLN
1	D	263	LYS
1	D	265	LEU
1	D	274	LEU
1	D	305	LEU
1	D	316	ARG
1	D	323	ARG
1	D	324	ILE
1	D	326	ARG
1	D	332	HIS
1	D	342	ILE

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Mol	Chain	Res	Type
1	E	104	LEU
1	E	120	LEU
1	E	129	GLU
1	E	151	LEU
1	E	188	ASN
1	E	202	VAL
1	E	213	LEU
1	E	251	ARG
1	E	257	ARG
1	E	261	LEU
1	E	263	LYS
1	E	265	LEU
1	E	274	LEU
1	E	304	ILE
1	E	305	LEU
1	E	324	ILE
1	E	332	HIS
1	E	342	ILE
1	E	349	ASP
1	F	99	ARG
1	F	105	LYS
1	F	109	THR
1	F	117	SER
1	F	129	GLU
1	F	151	LEU
1	F	184	GLU
1	F	202	VAL
1	F	204	ARG
1	F	213	LEU
1	F	214	LEU
1	F	261	LEU
1	F	265	LEU
1	F	274	LEU
1	F	286	GLN
1	F	307	HIS
1	F	324	ILE
1	F	329	ASP
1	F	332	HIS
1	F	342	ILE
1	G	97	PHE
1	G	99	ARG
1	G	124	LEU

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Mol	Chain	Res	Type
1	G	129	GLU
1	G	151	LEU
1	G	160	GLU
1	G	185	ILE
1	G	202	VAL
1	G	223	LYS
1	G	229	ASP
1	G	261	LEU
1	G	265	LEU
1	G	274	LEU
1	G	286	GLN
1	G	305	LEU
1	G	316	ARG
1	G	324	ILE
1	G	332	HIS
1	G	335	GLU
1	G	342	ILE
1	G	349	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	93	ASN
1	A	146	GLN
1	A	165	ASN
1	A	187	GLN
1	A	188	ASN
1	A	199	HIS
1	A	216	GLN
1	A	243	HIS
1	A	264	HIS
1	A	283	ASN
1	A	286	GLN
1	B	146	GLN
1	B	165	ASN
1	B	243	HIS
1	B	258	GLN
1	B	264	HIS
1	B	273	ASN
1	B	283	ASN
1	C	146	GLN

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Mol	Chain	Res	Type
1	C	165	ASN
1	C	187	GLN
1	C	211	GLN
1	C	273	ASN
1	C	283	ASN
1	C	286	GLN
1	D	146	GLN
1	D	165	ASN
1	D	187	GLN
1	D	199	HIS
1	D	227	ASN
1	D	264	HIS
1	D	273	ASN
1	D	283	ASN
1	D	286	GLN
1	D	303	HIS
1	E	146	GLN
1	E	165	ASN
1	E	264	HIS
1	E	273	ASN
1	E	283	ASN
1	E	284	GLN
1	E	286	GLN
1	E	303	HIS
1	F	146	GLN
1	F	165	ASN
1	F	188	ASN
1	F	211	GLN
1	F	227	ASN
1	F	258	GLN
1	F	273	ASN
1	F	283	ASN
1	F	286	GLN
1	F	332	HIS
1	G	146	GLN
1	G	165	ASN
1	G	187	GLN
1	G	211	GLN
1	G	217	GLN
1	G	227	ASN
1	G	273	ASN
1	G	283	ASN

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Mol	Chain	Res	Type
1	G	284	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](#)

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	G	378	-	7,7,7	0.68	0	9,10,10	0.50	0
3	IMD	F	363	-	5,5,5	1.25	1 (20%)	5,5,5	0.11	0
3	IMD	B	365	-	5,5,5	1.31	1 (20%)	5,5,5	0.34	0
3	IMD	A	364	-	5,5,5	1.41	1 (20%)	5,5,5	0.25	0
4	GOL	C	370	-	5,5,5	4.62	4 (80%)	5,5,5	5.98	3 (60%)
4	GOL	F	372	-	5,5,5	4.80	5 (100%)	5,5,5	6.08	3 (60%)
2	SO4	D	353	-	4,4,4	0.46	0	6,6,6	0.71	0
3	IMD	A	357	-	5,5,5	0.97	0	5,5,5	0.21	0
3	IMD	A	358	-	5,5,5	1.10	1 (20%)	5,5,5	0.19	0
5	MPD	E	376	-	7,7,7	0.63	0	9,10,10	0.62	0
2	SO4	E	354	-	4,4,4	0.37	0	6,6,6	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	F	366	-	5,5,5	4.95	5 (100%)	5,5,5	6.13	3 (60%)
4	GOL	B	367	-	5,5,5	4.71	5 (100%)	5,5,5	6.07	3 (60%)
2	SO4	C	352	-	4,4,4	0.51	0	6,6,6	0.70	0
3	IMD	A	361	-	5,5,5	1.31	1 (20%)	5,5,5	0.30	0
4	GOL	E	371	-	5,5,5	4.91	5 (100%)	5,5,5	6.03	3 (60%)
3	IMD	B	359	-	5,5,5	0.92	0	5,5,5	0.18	0
5	MPD	G	377	-	7,7,7	0.65	0	9,10,10	0.52	0
2	SO4	A	350	-	4,4,4	0.32	0	6,6,6	0.65	0
3	IMD	C	362	-	5,5,5	1.50	1 (20%)	5,5,5	0.33	0
2	SO4	B	351	-	4,4,4	0.46	0	6,6,6	0.75	0
5	MPD	B	375	-	7,7,7	0.59	0	9,10,10	0.56	0
4	GOL	C	368	-	5,5,5	4.79	5 (100%)	5,5,5	6.05	3 (60%)
3	IMD	B	360	-	5,5,5	1.15	1 (20%)	5,5,5	0.29	0
4	GOL	F	373	-	5,5,5	4.60	5 (100%)	5,5,5	6.18	3 (60%)
4	GOL	D	369	-	5,5,5	4.97	5 (100%)	5,5,5	6.17	3 (60%)
2	SO4	G	356	-	4,4,4	0.51	0	6,6,6	0.55	0
2	SO4	F	355	-	4,4,4	0.42	0	6,6,6	0.65	0
4	GOL	A	374	-	5,5,5	4.79	5 (100%)	5,5,5	5.94	3 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	G	378	-	-	0/5/5/5	-
3	IMD	F	363	-	-	-	0/1/1/1
3	IMD	B	365	-	-	-	0/1/1/1
3	IMD	A	364	-	-	-	0/1/1/1
4	GOL	C	370	-	-	2/4/4/4	-
4	GOL	F	372	-	-	3/4/4/4	-
3	IMD	A	357	-	-	-	0/1/1/1
3	IMD	A	358	-	-	-	0/1/1/1
5	MPD	E	376	-	-	1/5/5/5	-
4	GOL	F	366	-	-	2/4/4/4	-
4	GOL	B	367	-	-	2/4/4/4	-
3	IMD	A	361	-	-	-	0/1/1/1
4	GOL	E	371	-	-	2/4/4/4	-
3	IMD	B	359	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	G	377	-	-	0/5/5/5	-
3	IMD	C	362	-	-	-	0/1/1/1
5	MPD	B	375	-	-	0/5/5/5	-
4	GOL	C	368	-	-	3/4/4/4	-
4	GOL	F	373	-	-	2/4/4/4	-
3	IMD	B	360	-	-	-	0/1/1/1
4	GOL	D	369	-	-	3/4/4/4	-
4	GOL	A	374	-	-	3/4/4/4	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	366	GOL	C3-C2	-8.27	1.20	1.51
4	E	371	GOL	C3-C2	-8.20	1.20	1.51
4	C	368	GOL	C3-C2	-7.97	1.21	1.51
4	B	367	GOL	C3-C2	-7.93	1.21	1.51
4	A	374	GOL	C3-C2	-7.91	1.21	1.51
4	D	369	GOL	C3-C2	-7.86	1.21	1.51
4	C	370	GOL	C3-C2	-7.78	1.22	1.51
4	F	372	GOL	C3-C2	-7.73	1.22	1.51
4	F	373	GOL	C3-C2	-7.47	1.23	1.51
4	F	373	GOL	O1-C1	5.51	1.65	1.42
4	D	369	GOL	O1-C1	5.20	1.64	1.42
4	C	370	GOL	O1-C1	4.85	1.62	1.42
4	F	372	GOL	O1-C1	4.83	1.62	1.42
4	A	374	GOL	O1-C1	4.73	1.62	1.42
4	E	371	GOL	O1-C1	4.72	1.62	1.42
4	F	366	GOL	O1-C1	4.63	1.61	1.42
4	C	368	GOL	O1-C1	4.49	1.61	1.42
4	B	367	GOL	O1-C1	4.38	1.60	1.42
4	D	369	GOL	O2-C2	-3.93	1.32	1.43
4	B	367	GOL	O3-C3	3.73	1.58	1.42
4	F	366	GOL	O2-C2	-3.63	1.32	1.43
4	A	374	GOL	O3-C3	3.62	1.57	1.42
4	E	371	GOL	C1-C2	-3.51	1.38	1.51
4	F	372	GOL	O3-C3	3.51	1.57	1.42
4	F	372	GOL	C1-C2	-3.48	1.38	1.51
4	A	374	GOL	C1-C2	-3.46	1.38	1.51
4	C	368	GOL	C1-C2	-3.40	1.38	1.51
4	C	368	GOL	O3-C3	3.35	1.56	1.42
4	C	370	GOL	O3-C3	3.33	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	366	GOL	C1-C2	-3.31	1.39	1.51
4	E	371	GOL	O3-C3	3.26	1.56	1.42
4	D	369	GOL	O3-C3	3.23	1.56	1.42
4	F	373	GOL	O3-C3	3.04	1.55	1.42
4	F	366	GOL	O3-C3	2.96	1.54	1.42
4	D	369	GOL	C1-C2	-2.92	1.40	1.51
4	C	368	GOL	O2-C2	-2.83	1.35	1.43
4	E	371	GOL	O2-C2	-2.82	1.35	1.43
4	C	370	GOL	C1-C2	-2.77	1.41	1.51
4	B	367	GOL	O2-C2	-2.75	1.35	1.43
4	B	367	GOL	C1-C2	-2.73	1.41	1.51
4	F	372	GOL	O2-C2	-2.72	1.35	1.43
3	C	362	IMD	C5-N1	2.72	1.45	1.35
4	F	373	GOL	C1-C2	-2.51	1.42	1.51
3	A	364	IMD	C5-N1	2.48	1.44	1.35
3	B	365	IMD	C5-N1	2.45	1.44	1.35
3	A	361	IMD	C5-N1	2.39	1.44	1.35
3	B	360	IMD	C5-N1	2.23	1.43	1.35
4	A	374	GOL	O2-C2	-2.18	1.37	1.43
3	F	363	IMD	C5-N1	2.15	1.43	1.35
3	A	358	IMD	C5-N1	2.07	1.43	1.35
4	F	373	GOL	O2-C2	-2.06	1.37	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	373	GOL	O3-C3-C2	11.36	161.54	110.38
4	D	369	GOL	O3-C3-C2	11.16	160.61	110.38
4	F	366	GOL	O3-C3-C2	11.05	160.14	110.38
4	E	371	GOL	O3-C3-C2	11.02	159.98	110.38
4	C	368	GOL	O3-C3-C2	10.96	159.73	110.38
4	F	372	GOL	O3-C3-C2	10.96	159.72	110.38
4	B	367	GOL	O3-C3-C2	10.94	159.65	110.38
4	A	374	GOL	O3-C3-C2	10.91	159.50	110.38
4	C	370	GOL	O3-C3-C2	10.73	158.66	110.38
4	F	372	GOL	O2-C2-C3	7.43	139.93	109.18
4	D	369	GOL	O2-C2-C3	7.21	139.04	109.18
4	F	366	GOL	O2-C2-C3	7.21	139.02	109.18
4	C	370	GOL	O2-C2-C3	7.20	138.98	109.18
4	B	367	GOL	O2-C2-C3	7.12	138.66	109.18
4	C	368	GOL	O2-C2-C3	7.12	138.65	109.18
4	A	374	GOL	O2-C2-C3	7.10	138.59	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	371	GOL	O2-C2-C3	7.10	138.57	109.18
4	F	373	GOL	O2-C2-C3	6.90	137.74	109.18
4	D	369	GOL	O1-C1-C2	3.66	126.86	110.38
4	F	366	GOL	O1-C1-C2	3.56	126.41	110.38
4	B	367	GOL	O1-C1-C2	3.52	126.23	110.38
4	F	373	GOL	O1-C1-C2	3.47	125.98	110.38
4	C	368	GOL	O1-C1-C2	3.40	125.66	110.38
4	C	370	GOL	O1-C1-C2	3.26	125.05	110.38
4	F	372	GOL	O1-C1-C2	3.08	124.25	110.38
4	E	371	GOL	O1-C1-C2	3.06	124.16	110.38
4	A	374	GOL	O1-C1-C2	2.55	121.87	110.38

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	374	GOL	C1-C2-C3-O3
4	B	367	GOL	C1-C2-C3-O3
4	C	368	GOL	C1-C2-C3-O3
4	C	370	GOL	C1-C2-C3-O3
4	D	369	GOL	O1-C1-C2-C3
4	D	369	GOL	C1-C2-C3-O3
4	E	371	GOL	C1-C2-C3-O3
4	F	366	GOL	O1-C1-C2-C3
4	F	366	GOL	C1-C2-C3-O3
4	F	372	GOL	C1-C2-C3-O3
4	F	373	GOL	O1-C1-C2-O2
4	F	373	GOL	C1-C2-C3-O3
4	B	367	GOL	O1-C1-C2-O2
4	A	374	GOL	O1-C1-C2-C3
4	C	368	GOL	O1-C1-C2-C3
4	C	370	GOL	O1-C1-C2-O2
4	E	371	GOL	O1-C1-C2-O2
4	A	374	GOL	O1-C1-C2-O2
4	C	368	GOL	O1-C1-C2-O2
4	F	372	GOL	O1-C1-C2-O2
5	E	376	MPD	C1-C2-C3-C4
4	F	372	GOL	O1-C1-C2-C3
4	D	369	GOL	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	363	IMD	2	0
4	B	367	GOL	1	0
2	C	352	SO4	1	0
3	A	361	IMD	2	0
3	B	359	IMD	6	0
2	A	350	SO4	1	0
4	C	368	GOL	1	0
3	B	360	IMD	2	0
4	F	373	GOL	2	0
4	D	369	GOL	2	0
2	G	356	SO4	1	0
2	F	355	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	297/349 (85%)	0.21	4 (1%) 75 68	28, 66, 110, 161	0
1	B	236/349 (67%)	0.36	6 (2%) 58 49	32, 74, 132, 170	0
1	C	236/349 (67%)	0.55	10 (4%) 40 32	39, 78, 137, 198	0
1	D	236/349 (67%)	0.58	7 (2%) 52 44	41, 86, 139, 175	0
1	E	236/349 (67%)	0.27	9 (3%) 44 35	30, 62, 116, 197	0
1	F	236/349 (67%)	0.56	13 (5%) 30 23	37, 75, 121, 177	0
1	G	235/349 (67%)	0.58	15 (6%) 25 19	41, 82, 138, 190	0
All	All	1712/2443 (70%)	0.44	64 (3%) 45 35	28, 74, 133, 198	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	250	GLY	4.7
1	F	345	LYS	3.7
1	C	250	GLY	3.6
1	G	250	GLY	3.4
1	A	307	HIS	3.3
1	C	333	LEU	3.2
1	G	347	ILE	3.1
1	G	158	PRO	2.9
1	E	190	GLY	2.9
1	E	304	ILE	2.9
1	C	303	HIS	2.8
1	F	305	LEU	2.8
1	E	321	GLY	2.8
1	E	307	HIS	2.7
1	F	304	ILE	2.6
1	F	346	GLY	2.6
1	F	206	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	186	ALA	2.6
1	F	245	ARG	2.5
1	F	96	THR	2.5
1	G	191	LEU	2.5
1	E	305	LEU	2.4
1	G	304	ILE	2.4
1	D	96	THR	2.4
1	G	307	HIS	2.4
1	D	305	LEU	2.4
1	G	251	ARG	2.4
1	G	321	GLY	2.4
1	B	349	ASP	2.4
1	G	332	HIS	2.4
1	D	167	SER	2.3
1	E	96	THR	2.3
1	E	318	GLY	2.3
1	F	250	GLY	2.3
1	C	276	ASP	2.3
1	F	347	ILE	2.3
1	B	348	GLU	2.3
1	F	306	ALA	2.3
1	B	332	HIS	2.3
1	C	347	ILE	2.3
1	C	331	PRO	2.2
1	F	330	ALA	2.2
1	G	333	LEU	2.2
1	G	252	GLY	2.2
1	G	340	PHE	2.2
1	G	337	GLU	2.2
1	D	333	LEU	2.2
1	B	304	ILE	2.1
1	D	307	HIS	2.1
1	D	332	HIS	2.1
1	C	218	ALA	2.1
1	C	348	GLU	2.1
1	G	303	HIS	2.1
1	C	345	LYS	2.1
1	A	321	GLY	2.1
1	F	321	GLY	2.1
1	D	310	THR	2.1
1	E	303	HIS	2.1
1	B	321	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	324	ILE	2.1
1	G	276	ASP	2.0
1	B	339	VAL	2.0
1	A	349	ASP	2.0
1	F	335	GLU	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
3	IMD	A	361	5/5	0.54	0.23	119,119,119,119	0
3	IMD	B	365	5/5	0.59	0.19	92,92,92,92	0
5	MPD	G	377	8/8	0.59	0.15	106,106,106,106	0
4	GOL	E	371	6/6	0.62	0.11	66,66,66,66	0
4	GOL	F	373	6/6	0.66	0.09	88,88,88,88	0
3	IMD	A	364	5/5	0.67	0.19	93,93,93,93	0
3	IMD	B	360	5/5	0.68	0.20	81,81,81,81	0
3	IMD	A	358	5/5	0.76	0.26	101,101,101,101	0
4	GOL	A	374	6/6	0.76	0.11	76,76,76,76	0
4	GOL	B	367	6/6	0.76	0.13	68,68,68,68	0
3	IMD	C	362	5/5	0.78	0.15	94,94,94,94	0
4	GOL	C	368	6/6	0.78	0.11	77,77,77,77	0
4	GOL	C	370	6/6	0.78	0.13	88,88,88,88	0
5	MPD	E	376	8/8	0.79	0.14	84,84,84,84	0
3	IMD	F	363	5/5	0.79	0.14	100,100,100,100	0
4	GOL	F	372	6/6	0.80	0.09	76,76,76,76	0
5	MPD	G	378	8/8	0.82	0.13	112,112,112,112	0
3	IMD	A	357	5/5	0.83	0.15	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IMD	B	359	5/5	0.83	0.14	76,76,76,76	0
2	SO4	D	353	5/5	0.89	0.09	78,78,78,78	0
2	SO4	F	355	5/5	0.90	0.08	91,91,91,91	0
4	GOL	F	366	6/6	0.91	0.14	66,66,66,66	0
4	GOL	D	369	6/6	0.92	0.11	79,79,79,79	0
2	SO4	C	352	5/5	0.92	0.07	71,71,71,71	0
5	MPD	B	375	8/8	0.94	0.14	53,53,53,53	0
2	SO4	E	354	5/5	0.94	0.07	60,60,60,60	0
2	SO4	B	351	5/5	0.95	0.06	65,65,65,65	0
2	SO4	G	356	5/5	0.95	0.05	66,66,66,66	0
2	SO4	A	350	5/5	0.97	0.06	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.