



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:15 AM UTC

PDB ID : 1SXG / pdb_00001sxg
Title : Structural studies on the apo transcription factor form B. megaterium
Authors : Schumacher, M.A.; Allen, G.S.; Diel, M.; Seidel, G.; Hillen, W.; Brennan, R.G.
Deposited on : 2004-03-30
Resolution : 2.75 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:

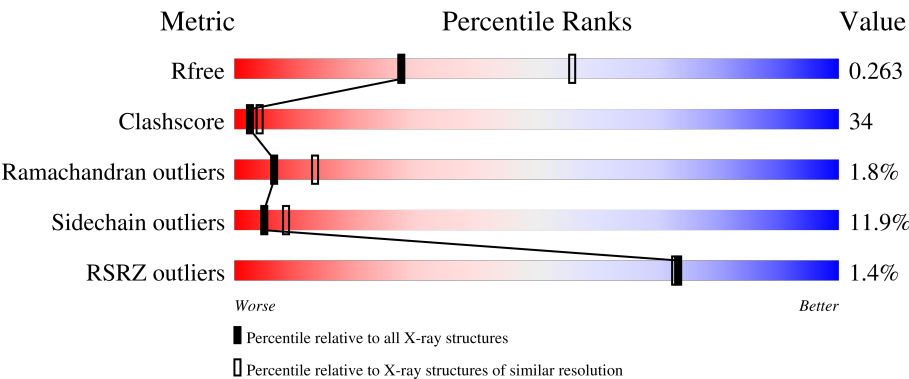
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	280	2% 46% 42% 9% ..
1	B	280	% 38% 47% 13% .
1	D	280	44% 42% 11% .
1	F	280	2% 44% 42% 11% .
1	I	280	2% 42% 43% 12% .

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Mol	Chain	Length	Quality of chain
1	P	280	% 38% 47% 12% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12939 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 Glucose-resistance amylase regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2141	1349	356	428	8			
1	D	273	Total	C	N	O	S	0	0	0
			2123	1337	352	426	8			
1	B	273	Total	C	N	O	S	0	0	0
			2123	1337	352	426	8			
1	I	275	Total	C	N	O	S	0	0	0
			2141	1349	356	428	8			
1	P	273	Total	C	N	O	S	0	0	0
			2123	1337	352	426	8			
1	F	273	Total	C	N	O	S	0	0	0
			2123	1337	352	426	8			

There are 18 discrepancies between the modelled and reference sequences:

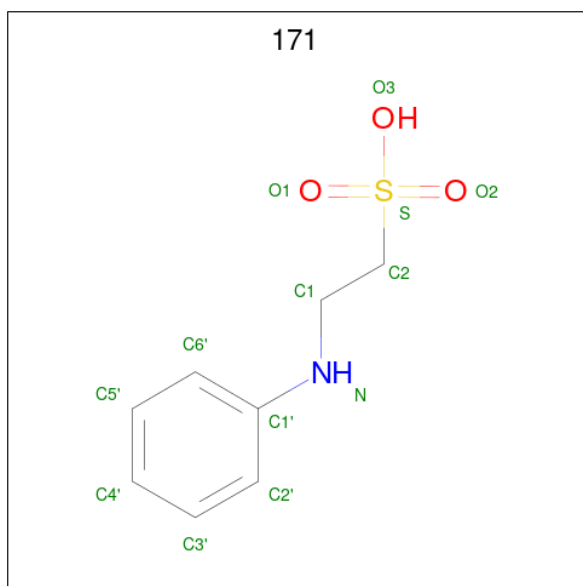
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	THR	SER	conflict	UNP P46828
A	105	GLU	GLN	conflict	UNP P46828
A	320	GLN	GLU	conflict	UNP P46828
D	87	THR	SER	conflict	UNP P46828
D	105	GLU	GLN	conflict	UNP P46828
D	320	GLN	GLU	conflict	UNP P46828
B	87	THR	SER	conflict	UNP P46828
B	105	GLU	GLN	conflict	UNP P46828
B	320	GLN	GLU	conflict	UNP P46828
I	87	THR	SER	conflict	UNP P46828
I	105	GLU	GLN	conflict	UNP P46828
I	320	GLN	GLU	conflict	UNP P46828
P	87	THR	SER	conflict	UNP P46828
P	105	GLU	GLN	conflict	UNP P46828
P	320	GLN	GLU	conflict	UNP P46828
F	87	THR	SER	conflict	UNP P46828
F	105	GLU	GLN	conflict	UNP P46828

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Chain	Residue	Modelled	Actual	Comment	Reference
F	320	GLN	GLU	conflict	UNP P46828

- Molecule 2 is 2-PHENYLAMINO-ETHANESULFONIC ACID (CCD ID: 171) (formula: $C_8H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

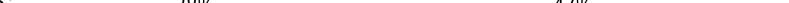
- Molecule 3 is water.

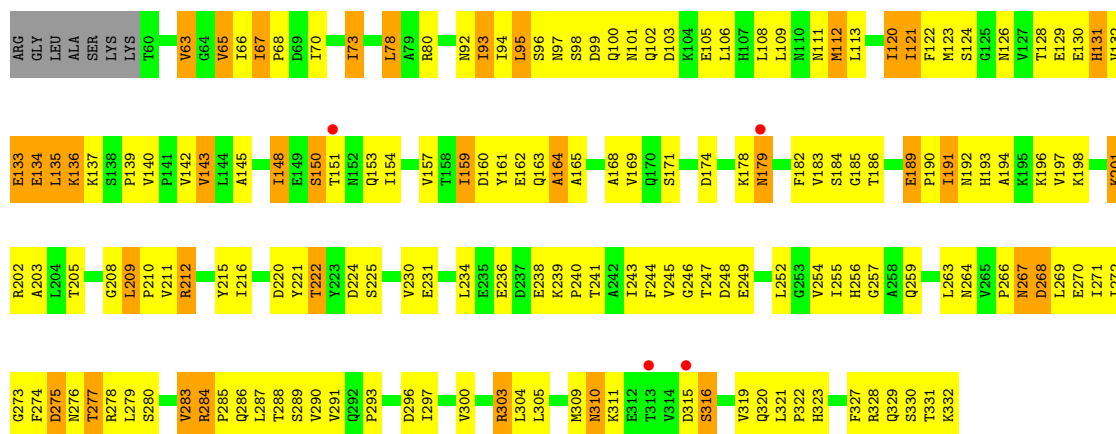
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	D	30	Total	O	0	0
			30	30		
3	B	24	Total	O	0	0
			24	24		
3	I	25	Total	O	0	0
			25	25		
3	P	17	Total	O	0	0
			17	17		
3	F	15	Total	O	0	0
			15	15		

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.

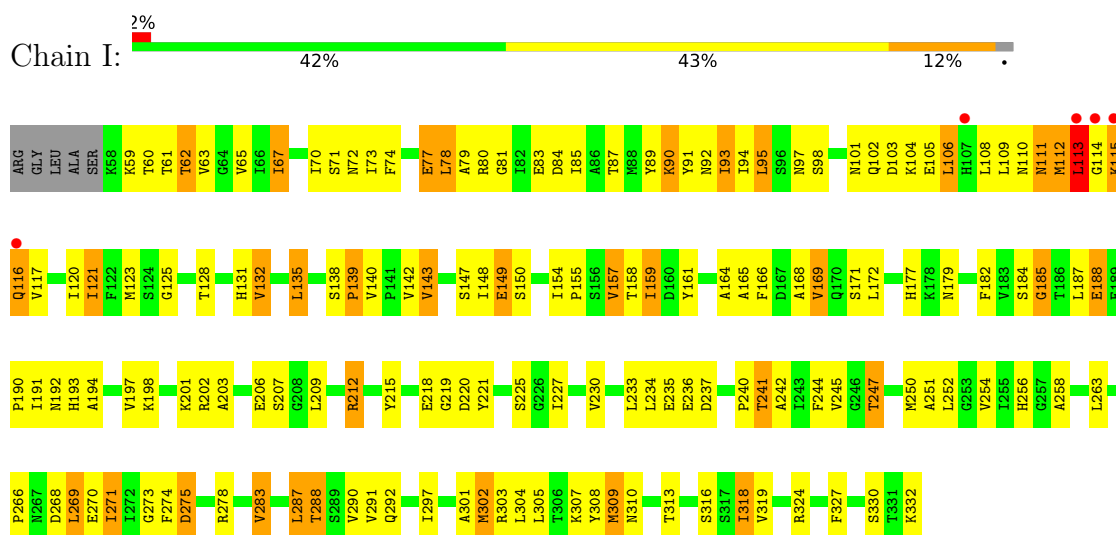
- Chain A:
-
- 2% 46% 42% 9% ..
- ARG GLY LEU ALA SER K58 K59 T60 T61 V62 V63 G64 V65 I66 I67 P68 D69 I70 S71 N72 I73 A76 E77 L78 R80 A79 D84 I85 A86 Y89 K90 Y91 N92 I93 I94 S96 N97 Q100 N101 Q102 D103 L108 M112 L113 G114 G115 Q116 V117 I121 F122 G125 T128 H131 V132 E133 E134 L135 K136 P139 V140 F141 V142 V143 A146 S147 I148 E149 S150 T151 N152 Q153 I154 V157 T158 I159 D160 T161 E162 Q163 E164 A165 F166 D167 A168 V169 Q170 S171 L172 I173 D174 S175 G176 H177 K178 M179 I180 A181 F182 V183 S184 G185 T186 L187 E188 P189 I191 N192 H193 A194 K195 K196 V197 Y200 K201 K202 A203 L204 T205 L209 R212 Y215 T216 V217 S225 G226 I227 E228 A229 V230 E231 K232 L233 E235 E236 D237 G246 T247 D248 F249 D250 A251 L252 G253 G254 I255 Q259 I271 I272 G273 F274 D275 M282 V283 R284 L287 L288 S289 V290 K293 K294 T295 D296 I297 V300 R303 L304 L305 T306 K307 M308 M309 V314 D315 S316 S317 I318 V319 Q320 L321 P322 F327 R328 Q329 S330 T331 K332

- [illegible]

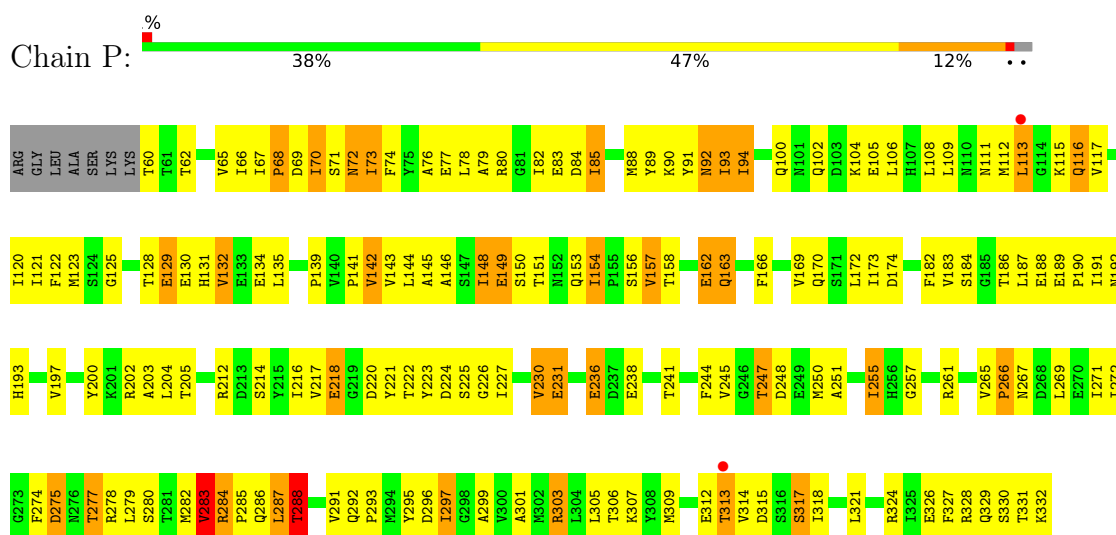
- Chain B:  38% 47% 13%



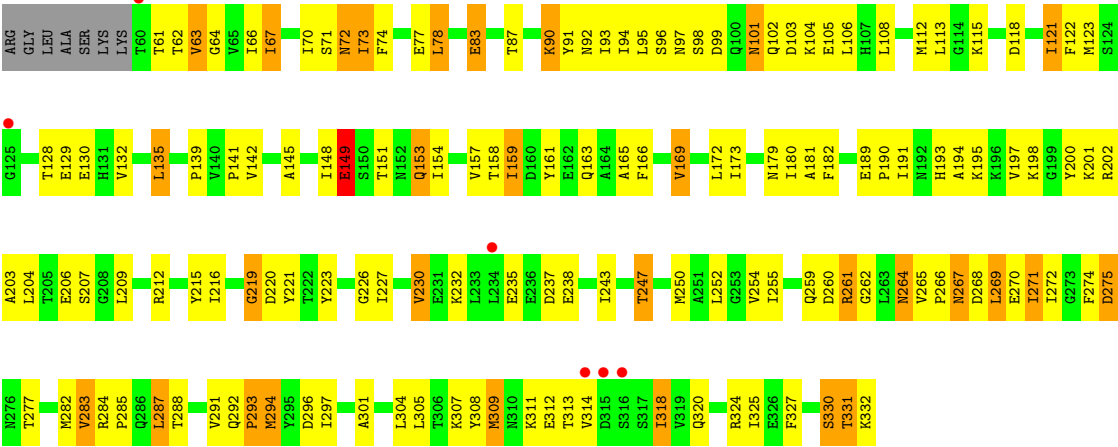
• Molecule 1: Glucose-resistance amylase regulator



• Molecule 1: Glucose-resistance amylase regulator



• Molecule 1: Glucose-resistance amylase regulator



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	375.39Å 60.14Å 75.65Å 90.00° 95.59° 90.00°	Depositor
Resolution (Å)	75.29 – 2.75 75.29 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (75.29-2.75) 99.0 (75.29-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.263 0.215 , 0.263	Depositor DCC
R_{free} test set	4413 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12939	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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:
171

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	0.61	1/2174 (0.0%)	1.10	14/2945 (0.5%)
1	B	0.55	0/2156	1.09	15/2923 (0.5%)
1	D	0.59	0/2156	1.12	17/2923 (0.6%)
1	F	0.56	0/2156	1.06	9/2923 (0.3%)
1	I	0.57	0/2174	1.13	19/2945 (0.6%)
1	P	0.55	0/2156	1.08	16/2923 (0.5%)
All	All	0.57	1/12972 (0.0%)	1.10	90/17582 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	MET	SD-CE	-7.31	1.61	1.79

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	ILE	CA-C-N	-7.91	112.01	120.47
1	D	67	ILE	C-N-CA	-7.91	112.01	120.47
1	B	121	ILE	N-CA-C	-7.72	97.32	108.36
1	B	134	GLU	N-CA-C	7.44	119.29	111.03
1	I	236	GLU	N-CA-C	-7.32	101.08	110.53
1	I	113	LEU	N-CA-C	-7.25	103.38	111.28
1	A	89	TYR	N-CA-C	-7.07	104.12	112.89
1	D	287	LEU	N-CA-C	6.88	119.70	109.59
1	P	265	VAL	N-CA-C	-6.88	99.43	107.61
1	A	288	THR	N-CA-C	-6.72	100.33	110.28
1	A	121	ILE	N-CA-C	-6.65	98.15	107.80
1	D	265	VAL	N-CA-C	-6.59	100.71	107.89
1	D	288	THR	N-CA-C	-6.52	99.28	109.25
1	B	231	GLU	N-CA-C	-6.48	104.22	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	150	SER	N-CA-C	6.47	118.88	111.11
1	P	292	GLN	N-CA-C	-6.39	96.90	109.10
1	P	317	SER	N-CA-C	6.35	119.50	111.69
1	I	125	GLY	N-CA-C	-6.34	105.77	114.64
1	D	227	ILE	N-CA-C	-6.33	104.58	110.53
1	I	227	ILE	N-CA-C	-6.24	104.43	110.42
1	F	149	GLU	N-CA-C	-6.12	105.62	114.12
1	B	131	HIS	N-CA-C	-6.11	104.54	111.14
1	B	209	LEU	CA-C-N	6.11	126.43	119.83
1	B	209	LEU	C-N-CA	6.11	126.43	119.83
1	A	235	GLU	N-CA-C	-6.11	105.69	113.02
1	A	69	ASP	N-CA-C	6.09	117.40	108.14
1	P	125	GLY	N-CA-C	-6.08	106.18	115.66
1	B	201	LYS	N-CA-C	-6.08	104.35	110.97
1	B	189	GLU	CA-C-N	5.91	127.23	119.84
1	B	189	GLU	C-N-CA	5.91	127.23	119.84
1	A	173	ILE	CB-CA-C	-5.86	104.47	111.97
1	I	319	VAL	N-CA-C	5.83	116.99	108.53
1	P	283	VAL	CB-CA-C	-5.82	103.21	111.19
1	B	130	GLU	N-CA-C	5.82	117.43	111.14
1	A	287	LEU	N-CA-C	5.82	118.15	109.25
1	I	93	ILE	N-CA-C	5.81	116.84	108.48
1	F	287	LEU	N-CA-C	5.80	118.65	110.23
1	I	120	ILE	N-CA-C	5.78	116.60	108.17
1	P	287	LEU	N-CA-C	5.77	118.08	109.25
1	I	148	ILE	N-CA-C	5.77	118.14	109.20
1	P	313	THR	N-CA-C	5.70	122.94	110.80
1	F	237	ASP	N-CA-C	-5.69	103.85	112.04
1	I	309	MET	N-CA-C	-5.68	106.39	113.15
1	D	219	GLY	N-CA-C	-5.66	104.81	112.57
1	F	291	VAL	N-CA-C	5.65	116.54	107.73
1	I	292	GLN	N-CA-C	-5.62	97.13	109.11
1	I	287	LEU	N-CA-C	5.61	119.07	110.20
1	F	153	GLN	N-CA-C	-5.58	104.59	111.40
1	P	288	THR	N-CA-C	-5.57	100.91	109.76
1	B	136	LYS	N-CA-C	-5.55	105.38	111.82
1	I	84	ASP	N-CA-C	-5.55	105.31	111.36
1	F	330	SER	N-CA-C	-5.50	105.83	112.54
1	I	185	GLY	N-CA-C	-5.48	103.59	112.31
1	P	92	ASN	N-CA-C	-5.48	101.87	110.36
1	I	288	THR	N-CA-C	-5.47	100.26	108.96
1	B	78	LEU	N-CA-C	-5.45	105.23	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	219	GLY	N-CA-C	-5.43	105.32	112.81
1	D	246	GLY	N-CA-C	5.42	119.24	112.73
1	B	289	SER	N-CA-C	5.41	117.61	109.23
1	B	164	ALA	N-CA-C	-5.39	105.49	111.36
1	D	330	SER	N-CA-C	-5.35	106.25	112.89
1	A	175	SER	N-CA-C	-5.32	106.75	113.18
1	A	255	ILE	CB-CA-C	-5.30	104.92	111.70
1	P	255	ILE	CB-CA-C	-5.29	104.93	111.70
1	A	173	ILE	N-CA-C	-5.26	105.36	110.42
1	A	250	MET	N-CA-C	-5.25	105.63	111.36
1	P	154	ILE	N-CA-C	-5.24	104.12	108.63
1	P	226	GLY	N-CA-C	-5.23	106.45	112.73
1	P	231	GLU	N-CA-C	-5.23	104.64	111.02
1	D	138	SER	CA-C-N	5.21	124.83	119.56
1	D	138	SER	C-N-CA	5.21	124.83	119.56
1	A	159	ILE	N-CA-C	-5.20	101.90	109.29
1	P	130	GLU	N-CA-C	-5.18	105.54	111.14
1	D	224	ASP	N-CA-C	5.17	116.73	111.14
1	D	261	ARG	N-CA-C	-5.17	106.65	113.17
1	A	150	SER	N-CA-C	5.15	121.77	110.80
1	I	159	ILE	N-CA-C	-5.15	102.54	108.82
1	F	267	ASN	N-CA-C	5.12	118.31	111.75
1	D	78	LEU	N-CA-C	-5.12	105.61	111.14
1	F	219	GLY	N-CA-C	-5.12	106.65	112.79
1	P	218	GLU	N-CA-C	5.10	117.87	109.76
1	D	173	ILE	CB-CA-C	-5.10	105.26	112.14
1	D	85	ILE	N-CA-C	-5.09	104.69	111.05
1	I	121	ILE	N-CA-C	-5.09	100.56	107.99
1	P	121	ILE	N-CA-C	-5.08	100.33	107.75
1	F	121	ILE	N-CA-C	-5.08	100.43	107.80
1	D	299	ALA	N-CA-C	-5.06	105.66	111.07
1	B	150	SER	N-CA-C	5.05	121.56	110.80
1	A	100	GLN	N-CA-C	5.02	118.37	111.54
1	I	291	VAL	N-CA-C	5.01	115.56	109.30

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	2141	0	2147	133	0
1	B	2123	0	2121	199	0
1	D	2123	0	2121	132	0
1	F	2123	0	2121	153	0
1	I	2141	0	2147	138	0
1	P	2123	0	2121	152	0
2	A	13	0	11	0	0
2	B	13	0	11	1	0
3	A	28	0	0	6	0
3	B	24	0	0	2	0
3	D	30	0	0	0	0
3	F	15	0	0	0	0
3	I	25	0	0	0	0
3	P	17	0	0	2	0
All	All	12939	0	12800	878	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 34.

All (878) 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:P:231:GLU:HG3	1:P:261:ARG:HH12	1.18	1.09
1:B:288:THR:HG22	1:B:328:ARG:H	1.12	1.08
1:A:305:LEU:HG	1:A:309:MET:HE2	1.36	1.04
1:B:191:ILE:HD12	1:B:191:ILE:H	1.22	1.01
1:F:277:THR:HG22	1:F:294:MET:HE1	1.42	1.00
1:A:252:LEU:HG	1:A:283:VAL:HG11	1.40	1.00
1:B:252:LEU:HG	1:B:283:VAL:HG13	1.46	0.97
1:B:277:THR:HG22	1:B:279:LEU:H	1.30	0.96
1:B:94:ILE:HD11	1:I:115:LYS:HE2	1.48	0.95
1:B:179:ASN:ND2	1:B:179:ASN:H	1.67	0.92
1:I:109:LEU:O	1:I:113:LEU:HD21	1.70	0.92
1:A:113:LEU:HD13	1:A:139:PRO:HG2	1.52	0.90
1:B:73:ILE:HD13	1:B:73:ILE:H	1.37	0.89
1:F:194:ALA:HA	1:F:198:LYS:HE2	1.54	0.89
1:P:113:LEU:HG	1:P:139:PRO:HG3	1.54	0.88
1:D:129:GLU:CD	1:D:129:GLU:H	1.83	0.87
1:B:222:THR:HG22	1:B:225:SER:H	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:ILE:HB	1:F:97:ASN:HD21	1.40	0.86
1:F:101:ASN:C	1:F:101:ASN:HD22	1.84	0.86
1:A:255:ILE:HD13	1:A:271:ILE:HD12	1.58	0.86
1:B:252:LEU:HG	1:B:283:VAL:CG1	2.06	0.85
1:A:80:ARG:NH2	1:D:97:ASN:HB3	1.91	0.85
1:P:182:PHE:CE1	1:P:184:SER:HB2	2.12	0.84
1:I:247:THR:HG22	1:I:250:MET:H	1.43	0.84
1:F:64:GLY:HA3	1:F:112:MET:HE2	1.60	0.84
1:F:307:LYS:HG2	1:F:314:VAL:HG22	1.59	0.83
1:B:288:THR:HG22	1:B:328:ARG:N	1.92	0.83
1:D:62:THR:HB	1:D:92:ASN:HB2	1.61	0.82
1:B:80:ARG:HD3	1:I:70:ILE:HG22	1.58	0.82
1:P:83:GLU:OE1	1:P:93:ILE:HG21	1.80	0.82
1:A:70:ILE:HG23	1:D:76:ALA:HB1	1.60	0.81
1:B:65:VAL:HB	1:B:95:LEU:HD22	1.62	0.81
1:B:142:VAL:HG13	1:B:154:ILE:HD11	1.62	0.81
1:P:94:ILE:HD11	1:F:94:ILE:HD12	1.63	0.81
1:F:148:ILE:HD11	1:F:190:PRO:HB2	1.60	0.81
1:P:85:ILE:HD12	1:P:299:ALA:HA	1.62	0.80
1:A:135:LEU:HD23	1:A:154:ILE:HG12	1.62	0.80
1:P:192:ASN:O	1:P:197:VAL:HG23	1.82	0.80
1:A:92:ASN:O	1:A:93:ILE:HD12	1.81	0.79
1:B:70:ILE:H	1:B:97:ASN:ND2	1.79	0.79
1:F:318:ILE:HD13	1:F:318:ILE:O	1.82	0.79
1:A:77:GLU:HB3	1:A:294:MET:HE1	1.65	0.79
1:A:296:ASP:HB3	1:A:321:LEU:HD13	1.63	0.79
1:I:303:ARG:HH12	1:I:307:LYS:HD2	1.45	0.79
1:A:80:ARG:HH22	1:D:97:ASN:HB3	1.45	0.78
1:B:112:MET:HG2	1:B:120:ILE:HD13	1.65	0.78
1:P:93:ILE:HG22	3:P:608:HOH:O	1.83	0.78
1:F:230:VAL:HG21	1:F:254:VAL:HA	1.65	0.77
1:B:179:ASN:H	1:B:179:ASN:HD22	1.31	0.77
1:F:247:THR:HG22	1:F:250:MET:H	1.49	0.77
1:A:288:THR:HB	1:A:327:PHE:HA	1.67	0.76
1:P:172:LEU:HD11	1:P:272:ILE:HD13	1.67	0.76
1:B:216:ILE:HG13	1:B:216:ILE:O	1.83	0.76
1:P:76:ALA:HB1	1:F:71:SER:HA	1.68	0.76
1:P:293:PRO:HB2	1:P:296:ASP:HB2	1.66	0.76
1:B:230:VAL:HG11	1:B:254:VAL:HG13	1.67	0.76
1:A:168:ALA:O	1:A:171:SER:HB3	1.86	0.75
1:B:277:THR:HG22	1:B:279:LEU:N	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLN:HG3	1:A:116:GLN:O	1.86	0.75
1:P:72:ASN:C	1:P:72:ASN:HD22	1.95	0.75
1:P:129:GLU:CD	1:P:129:GLU:H	1.94	0.75
1:P:277:THR:HG23	1:P:279:LEU:H	1.50	0.75
1:A:58:LYS:HD2	3:A:731:HOH:O	1.85	0.74
1:I:182:PHE:CE1	1:I:184:SER:HB2	2.21	0.74
1:P:287:LEU:HA	1:P:330:SER:OG	1.87	0.74
1:P:257:GLY:O	1:P:261:ARG:HD2	1.87	0.74
1:I:128:THR:H	1:I:131:HIS:HD2	1.35	0.74
1:P:288:THR:HG22	1:P:328:ARG:H	1.51	0.74
1:B:112:MET:HE3	1:B:112:MET:HA	1.69	0.73
1:B:135:LEU:HG	1:B:154:ILE:HD13	1.69	0.73
1:F:219:GLY:HA3	1:F:250:MET:HE1	1.70	0.73
1:B:288:THR:CG2	1:B:328:ARG:H	1.95	0.73
1:P:109:LEU:HD21	1:P:135:LEU:HD13	1.70	0.73
1:F:230:VAL:CG2	1:F:254:VAL:HA	2.18	0.73
1:A:216:ILE:HD13	1:A:216:ILE:O	1.88	0.73
1:P:151:THR:HG21	1:P:153:GLN:NE2	2.04	0.73
1:A:274:PHE:O	1:A:275:ASP:HB2	1.89	0.72
1:A:303:ARG:NH1	3:A:616:HOH:O	2.21	0.72
1:I:108:LEU:HA	1:I:111:ASN:HD22	1.53	0.72
1:B:230:VAL:CG1	1:B:254:VAL:HG13	2.19	0.72
1:A:288:THR:HG23	1:A:330:SER:OG	1.90	0.71
1:P:67:ILE:HD11	1:P:70:ILE:HD12	1.72	0.71
1:B:288:THR:HB	1:B:327:PHE:HA	1.72	0.71
1:P:172:LEU:HD21	1:P:272:ILE:HD11	1.71	0.71
1:B:182:PHE:HB3	1:B:216:ILE:HG22	1.72	0.70
1:A:68:PRO:HB3	1:A:100:GLN:NE2	2.07	0.70
1:I:157:VAL:HG22	1:I:297:ILE:HG23	1.72	0.70
1:P:73:ILE:O	1:P:77:GLU:HG3	1.92	0.70
1:A:293:PRO:O	1:A:297:ILE:HG12	1.92	0.69
1:B:277:THR:CG2	1:B:279:LEU:H	2.04	0.69
1:A:115:LYS:HD2	1:D:115:LYS:HB3	1.74	0.69
1:D:255:ILE:HG12	1:D:271:ILE:HD12	1.74	0.69
1:I:252:LEU:HG	1:I:283:VAL:CG1	2.23	0.69
1:F:271:ILE:HD11	1:F:287:LEU:HD13	1.75	0.69
1:D:126:ASN:HD22	1:D:190:PRO:HD3	1.58	0.69
1:A:68:PRO:HB3	1:A:100:GLN:HE22	1.57	0.68
1:I:252:LEU:HG	1:I:283:VAL:HG11	1.75	0.68
1:F:101:ASN:HD21	1:F:103:ASP:HB2	1.57	0.68
1:B:247:THR:HG22	1:B:249:GLU:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:GLU:CD	1:D:129:GLU:N	2.51	0.68
1:A:288:THR:HG22	1:A:328:ARG:H	1.59	0.68
1:F:157:VAL:HG11	1:F:301:ALA:HB2	1.75	0.67
1:D:255:ILE:O	1:D:259:GLN:HG3	1.94	0.67
1:I:135:LEU:HD23	1:I:154:ILE:HD12	1.76	0.67
1:P:291:VAL:HB	1:P:324:ARG:HG3	1.77	0.67
1:B:143:VAL:HG21	1:B:304:LEU:HD23	1.75	0.67
1:I:288:THR:HG23	1:I:327:PHE:HA	1.75	0.67
1:I:113:LEU:HD13	1:I:139:PRO:HD2	1.75	0.67
1:F:151:THR:HG22	1:F:153:GLN:HG2	1.77	0.67
1:B:70:ILE:HB	1:B:97:ASN:HD21	1.60	0.67
1:B:112:MET:HG2	1:B:120:ILE:CD1	2.25	0.67
1:I:77:GLU:OE2	1:I:278:ARG:HD3	1.94	0.67
1:B:70:ILE:CB	1:B:97:ASN:HD21	2.08	0.67
1:P:68:PRO:HB3	1:P:100:GLN:NE2	2.09	0.67
1:A:112:MET:HE3	1:A:117:VAL:HG11	1.77	0.66
1:A:288:THR:HG21	1:A:331:THR:OG1	1.94	0.66
1:D:129:GLU:HG2	1:D:130:GLU:OE2	1.96	0.66
1:F:197:VAL:HG22	1:F:201:LYS:HE3	1.77	0.66
1:D:212:ARG:HH12	1:D:238:GLU:HB2	1.60	0.66
1:B:191:ILE:H	1:B:191:ILE:CD1	2.02	0.66
1:I:303:ARG:NH1	1:I:307:LYS:HD2	2.10	0.66
1:A:172:LEU:HD11	1:A:272:ILE:HD13	1.78	0.66
1:D:288:THR:HG23	1:D:327:PHE:HA	1.78	0.66
1:I:302:MET:HE2	1:I:302:MET:HA	1.77	0.66
1:D:281:THR:HA	1:D:286:GLN:HE21	1.61	0.66
1:B:165:ALA:O	1:B:169:VAL:HG23	1.96	0.66
1:D:157:VAL:HG22	1:D:297:ILE:HG23	1.78	0.66
1:I:114:GLY:C	1:I:116:GLN:H	2.04	0.65
1:F:72:ASN:ND2	1:F:74:PHE:H	1.94	0.65
1:A:300:VAL:HG21	1:A:321:LEU:HD11	1.78	0.65
1:B:274:PHE:O	1:B:275:ASP:HB2	1.97	0.65
1:I:72:ASN:HD22	1:I:73:ILE:N	1.94	0.65
1:D:104:LYS:O	1:D:108:LEU:HG	1.96	0.65
1:I:318:ILE:HD13	1:I:318:ILE:O	1.97	0.65
1:P:274:PHE:O	1:P:275:ASP:HB2	1.96	0.65
1:F:72:ASN:HD22	1:F:73:ILE:N	1.94	0.65
1:D:109:LEU:HD21	1:D:135:LEU:HD13	1.78	0.65
1:D:151:THR:OG1	1:D:153:GLN:HG2	1.97	0.65
1:A:183:VAL:HG22	1:A:217:VAL:HG22	1.78	0.65
1:I:192:ASN:O	1:I:197:VAL:HG12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:ILE:HD11	1:F:95:LEU:HD21	1.79	0.64
1:D:226:GLY:O	1:D:230:VAL:HG23	1.97	0.64
1:B:151:THR:HG21	1:B:153:GLN:HE21	1.62	0.64
1:D:63:VAL:HG13	1:D:93:ILE:HD13	1.77	0.64
1:D:307:LYS:HD3	1:D:312:GLU:OE1	1.98	0.64
1:P:326:GLU:HG2	1:P:328:ARG:NH2	2.13	0.64
1:D:78:LEU:O	1:D:82:ILE:HG12	1.97	0.64
1:A:100:GLN:OE1	1:A:125:GLY:N	2.28	0.64
1:B:230:VAL:HG21	1:B:257:GLY:HA3	1.79	0.64
1:P:70:ILE:HD11	1:F:70:ILE:HG12	1.79	0.64
1:F:72:ASN:HD22	1:F:72:ASN:C	2.05	0.64
1:D:265:VAL:HG13	1:D:269:LEU:O	1.98	0.63
1:I:187:LEU:HD13	1:I:218:GLU:CG	2.29	0.63
1:I:215:TYR:CZ	1:I:240:PRO:HG3	2.34	0.63
1:A:230:VAL:CG2	1:A:254:VAL:HA	2.28	0.63
1:D:278:ARG:O	1:D:282:MET:HG3	1.99	0.63
1:I:81:GLY:O	1:I:85:ILE:HG12	1.98	0.63
1:I:305:LEU:HG	1:I:309:MET:HE2	1.81	0.63
1:F:72:ASN:ND2	1:F:73:ILE:HD13	2.13	0.63
1:A:308:TYR:CZ	1:A:314:VAL:HG21	2.33	0.63
1:D:123:MET:HE3	1:D:146:ALA:HB3	1.80	0.63
1:I:165:ALA:O	1:I:169:VAL:HG12	1.98	0.63
1:B:220:ASP:OD1	1:B:225:SER:HB3	1.98	0.63
1:I:270:GLU:CD	1:I:332:LYS:HB2	2.24	0.62
1:A:66:ILE:HG13	1:A:122:PHE:HD2	1.64	0.62
1:I:230:VAL:CG2	1:I:254:VAL:HA	2.29	0.62
1:F:165:ALA:O	1:F:169:VAL:HG12	1.99	0.62
1:A:112:MET:O	1:A:117:VAL:HG22	2.00	0.62
1:D:223:TYR:OH	1:D:256:HIS:HD2	1.81	0.62
1:P:94:ILE:HG12	1:F:94:ILE:HG23	1.81	0.62
1:A:92:ASN:C	1:A:93:ILE:HD12	2.24	0.62
1:D:182:PHE:CE1	1:D:184:SER:HB2	2.35	0.62
1:I:143:VAL:HB	1:I:155:PRO:HB2	1.81	0.62
1:B:182:PHE:CE1	1:B:184:SER:HB2	2.34	0.62
1:D:66:ILE:HB	1:D:122:PHE:HD2	1.65	0.62
1:P:286:GLN:HB2	1:P:329:GLN:NE2	2.15	0.62
1:B:111:ASN:ND2	1:I:92:ASN:ND2	2.47	0.61
1:I:94:ILE:HG21	1:I:112:MET:HE1	1.82	0.61
1:A:102:GLN:HG2	1:A:131:HIS:HE1	1.66	0.61
1:A:113:LEU:CD1	1:A:139:PRO:HG2	2.29	0.61
1:B:67:ILE:HG23	1:B:123:MET:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:128:THR:H	1:I:131:HIS:CD2	2.16	0.61
1:A:246:GLY:O	1:A:274:PHE:HB3	2.00	0.61
1:D:78:LEU:HB2	1:D:294:MET:HE3	1.83	0.61
1:D:85:ILE:HG21	1:D:302:MET:HB3	1.83	0.61
1:I:168:ALA:O	1:I:171:SER:HB3	1.99	0.61
1:P:89:TYR:HB3	1:P:91:TYR:CE2	2.36	0.61
1:P:283:VAL:O	1:P:284:ARG:HD2	2.01	0.61
1:B:143:VAL:HG12	1:B:305:LEU:HD13	1.82	0.61
1:P:90:LYS:O	1:P:90:LYS:HG3	2.00	0.61
1:F:202:ARG:O	1:F:206:GLU:HB3	2.01	0.61
1:F:227:ILE:O	1:F:230:VAL:HG23	2.01	0.60
1:A:284:ARG:NH1	1:D:256:HIS:HB3	2.16	0.60
1:D:123:MET:HG3	1:D:145:ALA:O	2.01	0.60
1:B:106:LEU:HD22	1:B:134:GLU:HG2	1.81	0.60
1:P:85:ILE:HD12	1:P:299:ALA:CA	2.29	0.60
1:D:83:GLU:O	1:D:86:ALA:HB3	2.01	0.60
1:I:67:ILE:HG22	1:I:123:MET:CE	2.32	0.60
1:I:230:VAL:HG12	1:I:234:LEU:HG	1.81	0.60
1:F:190:PRO:HA	1:F:193:HIS:CD2	2.36	0.60
1:D:121:ILE:HD11	1:D:302:MET:HG2	1.84	0.60
1:B:159:ILE:HG13	1:B:323:HIS:HB3	1.83	0.60
1:A:64:GLY:HA3	1:A:112:MET:HE2	1.83	0.60
1:A:108:LEU:O	1:A:112:MET:HG2	2.00	0.60
1:P:285:PRO:HB2	1:P:329:GLN:CB	2.32	0.60
1:F:252:LEU:HG	1:F:283:VAL:CG1	2.31	0.60
1:B:179:ASN:HD22	1:B:179:ASN:N	1.97	0.60
1:B:319:VAL:HG12	1:B:320:GLN:N	2.17	0.60
1:F:63:VAL:HG13	1:F:93:ILE:HD13	1.84	0.59
1:F:277:THR:HG22	1:F:294:MET:CE	2.26	0.59
1:A:180:ILE:HD12	1:A:204:LEU:HD21	1.83	0.59
1:B:65:VAL:HB	1:B:95:LEU:CD2	2.32	0.59
1:B:284:ARG:NH1	1:I:256:HIS:HB3	2.17	0.59
1:I:230:VAL:HG21	1:I:254:VAL:HA	1.83	0.59
1:F:172:LEU:HD21	1:F:272:ILE:CD1	2.32	0.59
1:P:274:PHE:O	1:P:275:ASP:CB	2.50	0.59
1:A:252:LEU:HG	1:A:283:VAL:CG1	2.25	0.59
1:B:159:ILE:HG12	1:B:160:ASP:N	2.17	0.59
1:I:112:MET:HE2	1:I:115:LYS:HD3	1.84	0.59
1:A:60:THR:HG21	1:A:92:ASN:OD1	2.03	0.59
1:D:227:ILE:HD13	1:D:253:GLY:O	2.03	0.59
1:I:113:LEU:HD13	1:I:139:PRO:CD	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:288:THR:HB	1:P:327:PHE:HA	1.84	0.59
1:A:62:THR:HG23	1:A:117:VAL:HA	1.85	0.59
1:P:170:GLN:NE2	1:P:174:ASP:OD1	2.36	0.59
1:F:118:ASP:O	1:F:141:PRO:HD2	2.02	0.59
1:A:153:GLN:O	1:A:154:ILE:HD12	2.03	0.59
1:D:267:ASN:HA	1:D:332:LYS:NZ	2.18	0.59
1:P:83:GLU:CD	1:P:93:ILE:HG21	2.28	0.59
1:P:288:THR:CG2	1:P:328:ARG:H	2.15	0.59
1:B:129:GLU:O	1:B:133:GLU:HG2	2.02	0.58
1:F:72:ASN:HD22	1:F:73:ILE:HD13	1.67	0.58
1:F:73:ILE:N	1:F:73:ILE:HD13	2.19	0.58
1:F:252:LEU:HG	1:F:283:VAL:HG11	1.84	0.58
1:A:71:SER:HB3	3:A:526:HOH:O	2.04	0.58
1:F:101:ASN:HD22	1:F:102:GLN:N	2.00	0.58
1:D:230:VAL:CG2	1:D:254:VAL:HA	2.34	0.58
1:I:270:GLU:OE1	1:I:332:LYS:HB2	2.03	0.58
1:P:85:ILE:CD1	1:P:299:ALA:HA	2.31	0.58
1:F:200:TYR:HE1	1:F:216:ILE:HD11	1.69	0.58
1:D:83:GLU:O	1:D:87:THR:HG23	2.03	0.58
1:F:260:ASP:C	1:F:262:GLY:H	2.11	0.58
1:A:228:GLU:O	1:A:232:LYS:HG3	2.04	0.58
1:I:67:ILE:HG22	1:I:123:MET:HE2	1.84	0.58
1:F:172:LEU:HD11	1:F:272:ILE:HD13	1.84	0.58
1:F:274:PHE:O	1:F:275:ASP:HB2	2.02	0.58
1:P:148:ILE:HD13	1:P:190:PRO:HB2	1.86	0.58
1:B:179:ASN:ND2	1:B:179:ASN:N	2.40	0.57
1:P:220:ASP:O	1:P:221:TYR:HB2	2.04	0.57
1:D:274:PHE:O	1:D:275:ASP:CG	2.47	0.57
1:I:121:ILE:CD1	1:I:305:LEU:HD22	2.34	0.57
1:F:194:ALA:O	1:F:198:LYS:HD2	2.05	0.57
1:F:62:THR:HA	1:F:92:ASN:HB2	1.85	0.57
1:B:178:LYS:HE3	1:B:210:PRO:HG2	1.86	0.57
1:A:80:ARG:HH11	1:A:80:ARG:HG2	1.69	0.57
1:B:67:ILE:HD11	1:B:95:LEU:HD11	1.86	0.57
1:F:123:MET:HG2	1:F:145:ALA:O	2.04	0.57
1:B:197:VAL:HG12	1:B:201:LYS:HE2	1.87	0.57
1:I:207:SER:HB3	1:I:209:LEU:HD12	1.86	0.57
1:P:113:LEU:C	1:P:113:LEU:HD13	2.30	0.57
1:P:288:THR:HG21	1:P:331:THR:OG1	2.04	0.57
1:A:116:GLN:O	1:A:116:GLN:CG	2.52	0.56
1:D:224:ASP:O	1:D:228:GLU:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:N	1:B:97:ASN:ND2	2.50	0.56
1:P:129:GLU:HA	1:P:132:VAL:HG12	1.87	0.56
1:A:160:ASP:HB2	1:A:320:GLN:CD	2.30	0.56
1:A:80:ARG:HG2	1:A:80:ARG:NH1	2.20	0.56
1:I:182:PHE:HD2	1:I:244:PHE:O	1.89	0.56
1:P:214:SER:HB2	1:P:236:GLU:OE2	2.05	0.56
1:F:67:ILE:HD13	1:F:67:ILE:H	1.71	0.56
1:F:70:ILE:H	1:F:97:ASN:ND2	2.03	0.56
1:B:136:LYS:HE3	1:B:153:GLN:HB3	1.87	0.56
1:B:128:THR:O	1:B:132:VAL:HG23	2.05	0.56
1:B:132:VAL:O	1:B:136:LYS:HB2	2.05	0.56
1:A:148:ILE:HG22	1:A:191:ILE:HG23	1.87	0.56
1:A:183:VAL:HG22	1:A:217:VAL:CG2	2.35	0.56
1:A:230:VAL:HG22	1:A:254:VAL:HA	1.88	0.56
1:I:65:VAL:HG13	1:I:95:LEU:HG	1.87	0.56
1:B:92:ASN:O	1:B:93:ILE:HD12	2.06	0.56
1:B:178:LYS:HG2	1:B:209:LEU:HD22	1.87	0.56
1:B:296:ASP:O	1:B:300:VAL:HG23	2.06	0.56
1:B:95:LEU:HD13	1:B:96:SER:N	2.21	0.56
1:B:160:ASP:OD2	1:B:163:GLN:HB2	2.07	0.55
1:F:128:THR:O	1:F:132:VAL:HG23	2.07	0.55
1:B:151:THR:HG21	1:B:153:GLN:NE2	2.21	0.55
1:B:191:ILE:HD12	1:B:191:ILE:N	2.07	0.55
1:I:110:ASN:HA	1:I:113:LEU:HD11	1.88	0.55
1:I:303:ARG:HG2	1:I:303:ARG:HH11	1.71	0.55
1:F:67:ILE:O	1:F:97:ASN:HA	2.07	0.55
1:P:172:LEU:HD21	1:P:272:ILE:CD1	2.35	0.55
1:F:274:PHE:O	1:F:275:ASP:CB	2.54	0.55
1:D:201:LYS:O	1:D:205:THR:HG23	2.06	0.55
1:B:273:GLY:N	1:B:287:LEU:HD11	2.21	0.55
1:F:98:SER:O	1:F:104:LYS:HD3	2.07	0.55
1:F:173:ILE:HD12	1:F:209:LEU:HD12	1.87	0.55
1:D:231:GLU:O	1:D:235:GLU:HG2	2.07	0.55
1:B:277:THR:CG2	1:B:278:ARG:N	2.70	0.55
1:I:187:LEU:HB2	1:I:218:GLU:OE2	2.06	0.55
1:I:59:LYS:HD2	1:I:60:THR:O	2.07	0.55
1:P:132:VAL:HG23	1:P:154:ILE:HG12	1.88	0.55
1:F:191:ILE:O	1:F:195:LYS:HB2	2.07	0.55
1:A:60:THR:CG2	1:A:92:ASN:OD1	2.55	0.55
1:I:269:LEU:HD13	1:I:271:ILE:CD1	2.36	0.55
1:B:182:PHE:CZ	1:B:184:SER:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:187:LEU:HD13	1:I:218:GLU:HG3	1.88	0.55
1:I:273:GLY:HA3	1:I:287:LEU:HD21	1.89	0.55
1:P:132:VAL:HA	1:P:135:LEU:HB3	1.88	0.55
1:D:65:VAL:HG22	1:D:95:LEU:HD12	1.88	0.55
1:D:126:ASN:HD22	1:D:190:PRO:CD	2.19	0.55
1:B:198:LYS:NZ	1:B:202:ARG:HD3	2.22	0.55
1:B:215:TYR:CZ	1:B:240:PRO:HG3	2.41	0.55
1:F:318:ILE:O	1:F:318:ILE:CD1	2.55	0.54
1:I:89:TYR:O	1:I:90:LYS:HD3	2.07	0.54
1:A:143:VAL:HG13	1:A:305:LEU:HD13	1.89	0.54
1:B:70:ILE:HD11	1:I:70:ILE:HG13	1.88	0.54
1:D:97:ASN:O	1:D:104:LYS:HE2	2.07	0.54
1:I:233:LEU:C	1:I:235:GLU:H	2.14	0.54
1:P:192:ASN:C	1:P:197:VAL:HG23	2.33	0.54
1:P:288:THR:HG23	1:P:330:SER:HB2	1.88	0.54
1:D:291:VAL:HG21	1:D:324:ARG:NH1	2.23	0.54
1:B:274:PHE:O	1:B:275:ASP:CB	2.55	0.54
1:P:293:PRO:CB	1:P:296:ASP:HB2	2.37	0.54
1:P:169:VAL:HG21	1:P:200:TYR:HA	1.89	0.54
1:B:230:VAL:O	1:B:234:LEU:HG	2.07	0.54
1:B:293:PRO:O	1:B:297:ILE:HG13	2.06	0.54
1:F:250:MET:O	1:F:254:VAL:HG23	2.07	0.54
1:F:288:THR:HG23	1:F:327:PHE:HA	1.90	0.54
1:D:164:ALA:HB1	1:D:290:VAL:HG11	1.89	0.54
1:B:230:VAL:HG13	1:B:254:VAL:HG22	1.90	0.54
1:I:128:THR:O	1:I:131:HIS:HB2	2.08	0.54
1:P:157:VAL:HG11	1:P:301:ALA:HB2	1.90	0.54
1:B:102:GLN:HG3	1:B:131:HIS:NE2	2.23	0.54
1:F:292:GLN:O	1:F:294:MET:N	2.40	0.54
1:A:69:ASP:HA	1:A:97:ASN:OD1	2.08	0.54
1:D:292:GLN:CG	1:D:292:GLN:O	2.56	0.54
1:P:156:SER:OG	1:P:318:ILE:HG23	2.08	0.54
1:D:169:VAL:O	1:D:173:ILE:HG12	2.07	0.53
1:B:255:ILE:HG12	1:B:271:ILE:HD13	1.90	0.53
1:I:72:ASN:C	1:I:72:ASN:ND2	2.65	0.53
1:P:151:THR:HG21	1:P:153:GLN:CD	2.33	0.53
1:P:318:ILE:N	1:P:318:ILE:HD12	2.22	0.53
1:B:101:ASN:O	1:B:105:GLU:HG3	2.08	0.53
1:I:78:LEU:HD13	1:I:123:MET:SD	2.48	0.53
1:I:135:LEU:HD23	1:I:154:ILE:CD1	2.38	0.53
1:P:112:MET:HB3	1:P:117:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:297:ILE:HD12	1:P:321:LEU:HD12	1.90	0.53
1:P:106:LEU:HD21	1:P:134:GLU:HB2	1.91	0.53
1:A:89:TYR:O	1:A:90:LYS:HB2	2.09	0.53
1:A:102:GLN:HG2	1:A:131:HIS:CE1	2.42	0.53
1:B:238:GLU:CD	1:B:238:GLU:H	2.16	0.53
1:I:94:ILE:CG2	1:I:112:MET:HE1	2.38	0.53
1:F:200:TYR:CE1	1:F:216:ILE:HD11	2.42	0.53
1:D:112:MET:HE2	1:D:112:MET:HA	1.90	0.53
1:P:285:PRO:HB2	1:P:329:GLN:HB2	1.91	0.53
1:I:113:LEU:H	1:I:113:LEU:CD2	2.15	0.53
1:D:66:ILE:HB	1:D:122:PHE:CD2	2.44	0.53
1:A:274:PHE:O	1:A:275:ASP:CB	2.57	0.53
1:D:184:SER:OG	1:D:185:GLY:N	2.39	0.53
1:B:120:ILE:H	1:B:305:LEU:HD11	1.72	0.53
1:B:288:THR:HG21	1:B:331:THR:OG1	2.08	0.53
1:F:212:ARG:NH1	1:F:238:GLU:HB2	2.23	0.53
1:B:220:ASP:OD1	1:B:222:THR:HB	2.08	0.53
1:B:70:ILE:H	1:B:97:ASN:HD22	1.57	0.52
1:P:247:THR:HG22	1:P:250:MET:H	1.74	0.52
1:F:264:ASN:H	1:F:268:ASP:HB2	1.73	0.52
1:B:284:ARG:HH21	1:B:286:GLN:HG3	1.74	0.52
1:A:68:PRO:CB	1:A:100:GLN:NE2	2.72	0.52
1:B:121:ILE:CD1	1:B:305:LEU:HD22	2.39	0.52
1:B:148:ILE:HG13	1:B:191:ILE:HG13	1.92	0.52
1:D:281:THR:CA	1:D:286:GLN:HE21	2.22	0.52
1:I:113:LEU:H	1:I:113:LEU:HD23	1.73	0.52
1:I:274:PHE:O	1:I:275:ASP:HB2	2.09	0.52
1:A:192:ASN:O	1:A:197:VAL:HG23	2.10	0.52
1:D:67:ILE:HD12	1:D:75:TYR:HB3	1.90	0.52
1:B:94:ILE:HG23	1:I:94:ILE:HG23	1.92	0.52
1:P:93:ILE:O	1:P:93:ILE:CG2	2.57	0.52
1:F:307:LYS:NZ	1:F:313:THR:O	2.35	0.52
1:D:157:VAL:HA	1:D:319:VAL:O	2.10	0.52
1:B:113:LEU:HD13	1:B:139:PRO:HD2	1.92	0.52
1:P:67:ILE:CD1	1:P:70:ILE:HD12	2.39	0.52
1:F:193:HIS:HD2	1:F:194:ALA:N	2.08	0.52
1:D:85:ILE:CD1	1:D:299:ALA:HB1	2.40	0.52
1:B:98:SER:CB	1:B:105:GLU:HG2	2.40	0.52
1:B:238:GLU:N	1:B:238:GLU:OE2	2.43	0.52
1:P:72:ASN:ND2	1:P:74:PHE:H	2.08	0.52
1:D:174:ASP:C	1:D:176:GLY:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:HA	3:A:552:HOH:O	2.10	0.51
1:B:126:ASN:ND2	1:B:190:PRO:HG2	2.25	0.51
1:B:211:VAL:HG12	1:B:211:VAL:O	2.09	0.51
1:A:148:ILE:HD13	1:A:148:ILE:C	2.36	0.51
1:B:267:ASN:HA	1:B:332:LYS:NZ	2.25	0.51
1:I:263:LEU:CD1	1:I:268:ASP:HB3	2.40	0.51
1:P:149:GLU:HG3	1:P:149:GLU:O	2.09	0.51
1:P:169:VAL:O	1:P:173:ILE:HG13	2.10	0.51
1:B:151:THR:CG2	1:B:153:GLN:HE21	2.24	0.51
1:I:263:LEU:HD11	1:I:268:ASP:HB3	1.92	0.51
1:I:266:PRO:HB2	1:I:270:GLU:HG2	1.92	0.51
1:P:255:ILE:HD13	1:P:271:ILE:HG13	1.92	0.51
1:D:302:MET:CE	1:D:305:LEU:HD23	2.40	0.51
1:I:89:TYR:O	1:I:90:LYS:CD	2.59	0.51
1:D:185:GLY:O	1:D:186:THR:C	2.53	0.51
1:F:73:ILE:HD13	1:F:73:ILE:H	1.76	0.51
1:D:85:ILE:HD11	1:D:299:ALA:HB1	1.92	0.51
1:D:128:THR:O	1:D:131:HIS:HB2	2.11	0.51
1:B:222:THR:HG23	1:B:224:ASP:H	1.74	0.51
1:P:78:LEU:O	1:P:82:ILE:HG12	2.11	0.51
1:P:128:THR:HB	1:P:129:GLU:OE1	2.10	0.51
1:F:172:LEU:HD21	1:F:272:ILE:HD11	1.92	0.51
1:B:73:ILE:HG13	1:B:279:LEU:HG	1.93	0.51
1:B:164:ALA:HB1	1:B:290:VAL:HG11	1.93	0.51
1:F:135:LEU:HD12	1:F:142:VAL:HG11	1.92	0.51
1:B:67:ILE:HG23	1:B:123:MET:CE	2.41	0.51
1:B:120:ILE:O	1:B:142:VAL:HA	2.11	0.51
1:B:212:ARG:NH2	1:B:238:GLU:HG3	2.26	0.51
1:F:101:ASN:O	1:F:105:GLU:HG3	2.11	0.51
1:D:66:ILE:HD13	1:D:96:SER:HB2	1.92	0.50
1:B:270:GLU:OE2	1:B:332:LYS:HB2	2.11	0.50
1:A:186:THR:HG22	1:A:188:GLU:CD	2.35	0.50
1:D:191:ILE:HG23	1:D:192:ASN:ND2	2.25	0.50
1:P:68:PRO:HB3	1:P:100:GLN:HE22	1.76	0.50
1:P:182:PHE:CZ	1:P:184:SER:HB2	2.45	0.50
1:D:146:ALA:HA	1:D:158:THR:HG22	1.93	0.50
1:B:112:MET:HA	1:B:112:MET:CE	2.39	0.50
1:I:72:ASN:HD22	1:I:72:ASN:C	2.17	0.50
1:I:169:VAL:HA	1:I:172:LEU:HD12	1.93	0.50
1:P:151:THR:HB	1:P:153:GLN:HG2	1.94	0.50
1:D:230:VAL:HG21	1:D:254:VAL:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:231:GLU:CG	1:P:261:ARG:HH12	2.06	0.50
1:A:228:GLU:HG3	1:A:232:LYS:HE3	1.92	0.50
1:I:149:GLU:OE1	1:I:154:ILE:HG12	2.11	0.50
1:F:62:THR:HG22	1:F:92:ASN:HB2	1.93	0.50
1:A:146:ALA:HA	1:A:158:THR:HG22	1.94	0.50
1:B:131:HIS:O	1:B:135:LEU:HD22	2.12	0.50
1:B:148:ILE:HD12	1:B:148:ILE:O	2.11	0.50
1:P:93:ILE:O	1:P:93:ILE:HG23	2.12	0.50
1:P:104:LYS:O	1:P:108:LEU:HG	2.12	0.50
1:D:66:ILE:HD12	1:D:108:LEU:HB3	1.94	0.50
1:B:112:MET:HB3	1:B:120:ILE:HD11	1.93	0.50
1:B:198:LYS:O	1:B:202:ARG:HG3	2.12	0.50
1:P:89:TYR:O	1:P:90:LYS:HG2	2.12	0.50
1:P:113:LEU:CG	1:P:139:PRO:HG3	2.36	0.50
1:P:324:ARG:NH2	1:P:326:GLU:OE1	2.45	0.50
1:B:95:LEU:HD13	1:B:96:SER:H	1.77	0.50
1:I:128:THR:O	1:I:132:VAL:HG12	2.12	0.50
1:B:215:TYR:CE2	1:B:240:PRO:HG3	2.47	0.50
1:F:77:GLU:HG3	1:F:294:MET:HE2	1.93	0.50
1:A:128:THR:O	1:A:132:VAL:HG23	2.12	0.49
1:A:300:VAL:CG2	1:A:321:LEU:HD11	2.42	0.49
1:D:163:GLN:NE2	1:D:202:ARG:HH22	2.10	0.49
1:D:234:LEU:O	1:D:239:LYS:HE2	2.12	0.49
1:B:70:ILE:H	1:B:97:ASN:HD21	1.58	0.49
1:I:157:VAL:HG11	1:I:301:ALA:HB2	1.92	0.49
1:P:307:LYS:HB3	1:P:312:GLU:HB2	1.93	0.49
1:D:230:VAL:HG22	1:D:254:VAL:HG13	1.93	0.49
1:F:149:GLU:OE1	1:F:151:THR:HB	2.11	0.49
1:B:238:GLU:O	1:B:238:GLU:HG2	2.12	0.49
1:I:287:LEU:HA	1:I:330:SER:HB3	1.94	0.49
1:P:285:PRO:HB2	1:P:329:GLN:HB3	1.93	0.49
1:F:197:VAL:HG13	1:F:198:LYS:N	2.26	0.49
1:B:70:ILE:CG2	1:B:97:ASN:HD21	2.25	0.49
1:A:162:GLU:OE2	1:A:202:ARG:NH1	2.42	0.49
1:A:248:ASP:O	1:A:251:ALA:HB3	2.11	0.49
1:B:65:VAL:HG13	1:B:121:ILE:HB	1.95	0.49
1:P:220:ASP:OD1	1:P:225:SER:HB3	2.13	0.49
1:B:264:ASN:OD1	1:B:264:ASN:C	2.55	0.49
1:P:66:ILE:HB	1:P:122:PHE:HD2	1.77	0.49
1:B:121:ILE:HD12	1:B:305:LEU:HD22	1.95	0.49
1:I:121:ILE:HD11	1:I:302:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:267:ASN:HA	1:P:332:LYS:HE3	1.95	0.49
1:F:271:ILE:CD1	1:F:287:LEU:HD13	2.42	0.49
1:I:182:PHE:CZ	1:I:184:SER:HB2	2.47	0.49
1:A:86:ALA:HB1	1:A:93:ILE:HD11	1.94	0.49
1:D:66:ILE:HD11	1:D:112:MET:HG3	1.94	0.49
1:F:101:ASN:C	1:F:101:ASN:ND2	2.56	0.49
1:F:101:ASN:ND2	1:F:103:ASP:N	2.60	0.49
1:F:108:LEU:O	1:F:112:MET:HG2	2.12	0.49
1:F:159:ILE:HD11	1:F:161:TYR:CD2	2.48	0.49
1:F:255:ILE:CD1	1:F:265:VAL:HG11	2.43	0.49
1:I:166:PHE:CE2	1:I:203:ALA:HA	2.48	0.48
1:A:179:ASN:HB2	1:A:215:TYR:HE2	1.78	0.48
1:B:101:ASN:HD21	1:B:103:ASP:HB2	1.78	0.48
1:B:212:ARG:O	1:B:215:TYR:HB2	2.13	0.48
1:B:264:ASN:O	1:B:268:ASP:HB2	2.13	0.48
1:I:62:THR:HB	1:I:92:ASN:HB2	1.94	0.48
1:I:164:ALA:HB1	1:I:290:VAL:HG11	1.95	0.48
1:I:197:VAL:HG22	1:I:201:LYS:HD3	1.95	0.48
1:P:162:GLU:HG3	1:P:163:GLN:N	2.28	0.48
1:P:251:ALA:O	1:P:255:ILE:HG12	2.11	0.48
1:F:216:ILE:HG22	1:F:216:ILE:O	2.11	0.48
1:A:148:ILE:HD12	1:A:190:PRO:CB	2.43	0.48
1:A:303:ARG:O	1:A:307:LYS:HG3	2.13	0.48
1:I:274:PHE:O	1:I:275:ASP:CB	2.61	0.48
1:F:62:THR:HG22	1:F:92:ASN:OD1	2.12	0.48
1:A:113:LEU:HD21	1:A:139:PRO:HD2	1.95	0.48
1:A:230:VAL:HG21	1:A:254:VAL:HA	1.95	0.48
1:I:101:ASN:ND2	1:I:103:ASP:HB2	2.28	0.48
1:P:223:TYR:CD2	1:F:282:MET:HG2	2.48	0.48
1:F:96:SER:OG	1:F:108:LEU:HD22	2.14	0.48
1:D:144:LEU:HG	1:D:154:ILE:HG21	1.95	0.48
1:B:196:LYS:O	1:B:197:VAL:C	2.57	0.48
1:B:277:THR:HG23	1:B:278:ARG:N	2.29	0.48
1:I:241:THR:C	1:I:269:LEU:HD23	2.38	0.48
1:A:288:THR:CG2	1:A:328:ARG:H	2.26	0.48
1:P:67:ILE:HD12	1:P:67:ILE:O	2.14	0.48
1:P:89:TYR:OH	1:P:303:ARG:HG2	2.14	0.48
1:F:94:ILE:HG21	1:F:112:MET:HE1	1.96	0.48
1:F:129:GLU:CD	1:F:130:GLU:H	2.22	0.48
1:D:123:MET:HE3	1:D:146:ALA:CB	2.42	0.48
1:D:261:ARG:HG3	1:D:261:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:204:LEU:O	1:P:205:THR:C	2.55	0.48
1:B:98:SER:HB2	1:B:105:GLU:HG2	1.96	0.48
1:B:99:ASP:O	1:B:100:GLN:HB2	2.13	0.48
1:P:106:LEU:HD11	1:P:134:GLU:OE1	2.14	0.48
1:P:112:MET:O	1:P:117:VAL:HG22	2.13	0.48
1:A:306:THR:HA	1:A:309:MET:HE3	1.94	0.48
1:I:269:LEU:HD13	1:I:271:ILE:HD11	1.96	0.48
1:P:314:VAL:HG12	1:P:315:ASP:O	2.14	0.48
1:F:166:PHE:CE2	1:F:203:ALA:HA	2.49	0.48
1:A:72:ASN:HA	3:A:505:HOH:O	2.13	0.47
1:B:183:VAL:HG23	1:B:243:ILE:HG21	1.95	0.47
1:B:197:VAL:CG1	1:B:201:LYS:HE2	2.44	0.47
1:D:129:GLU:O	1:D:132:VAL:HG22	2.13	0.47
1:A:62:THR:HB	1:A:92:ASN:HB2	1.97	0.47
1:B:111:ASN:ND2	1:I:92:ASN:HD22	2.11	0.47
1:P:102:GLN:NE2	1:P:128:THR:HG21	2.28	0.47
1:F:169:VAL:HG11	1:F:200:TYR:HA	1.96	0.47
1:D:288:THR:H	1:D:330:SER:HB3	1.80	0.47
1:I:101:ASN:HB3	1:I:104:LYS:HB2	1.95	0.47
1:P:288:THR:HG22	1:P:328:ARG:N	2.25	0.47
1:F:304:LEU:HD11	1:F:314:VAL:CG1	2.44	0.47
1:A:172:LEU:HD11	1:A:272:ILE:CD1	2.45	0.47
1:B:111:ASN:HD21	1:I:92:ASN:ND2	2.11	0.47
1:B:113:LEU:HD22	1:B:140:VAL:HG22	1.96	0.47
1:B:208:GLY:O	1:B:209:LEU:HD23	2.14	0.47
1:I:111:ASN:O	1:I:115:LYS:HD2	2.15	0.47
1:A:225:SER:O	1:A:228:GLU:HG2	2.15	0.47
1:D:302:MET:HE2	1:D:302:MET:HA	1.97	0.47
1:I:83:GLU:O	1:I:87:THR:HG23	2.13	0.47
1:F:158:THR:O	1:F:320:GLN:HA	2.15	0.47
1:A:76:ALA:HB1	1:D:71:SER:HA	1.96	0.47
1:A:94:ILE:HD11	1:D:115:LYS:NZ	2.30	0.47
1:A:157:VAL:HA	1:A:319:VAL:O	2.15	0.47
1:D:166:PHE:CD1	1:D:166:PHE:C	2.92	0.47
1:D:172:LEU:HD21	1:D:272:ILE:HD13	1.97	0.47
1:D:182:PHE:HE1	1:D:197:VAL:HG22	1.80	0.47
1:B:73:ILE:CD1	1:I:278:ARG:HH22	2.28	0.47
1:B:102:GLN:HG3	1:B:131:HIS:CE1	2.49	0.47
1:B:182:PHE:HD2	1:B:244:PHE:O	1.98	0.47
1:B:208:GLY:HA2	3:B:538:HOH:O	2.14	0.47
1:I:101:ASN:O	1:I:105:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:109:LEU:HD11	1:I:142:VAL:HG21	1.96	0.47
1:P:129:GLU:CD	1:P:129:GLU:N	2.70	0.47
1:P:187:LEU:O	1:P:193:HIS:HB3	2.15	0.47
1:P:189:GLU:HB2	1:P:191:ILE:HG22	1.96	0.47
1:F:308:TYR:O	1:F:311:LYS:N	2.34	0.47
1:P:69:ASP:OD2	1:P:71:SER:HB3	2.14	0.47
1:P:115:LYS:O	1:F:115:LYS:HE3	2.14	0.47
1:P:227:ILE:O	1:P:230:VAL:HG23	2.15	0.47
1:A:182:PHE:CE1	1:A:184:SER:HB3	2.50	0.47
1:D:106:LEU:HD22	1:D:110:ASN:HD21	1.79	0.47
1:D:202:ARG:O	1:D:206:GLU:HG3	2.14	0.47
1:B:246:GLY:O	1:B:274:PHE:HB3	2.15	0.47
1:I:308:TYR:C	1:I:310:ASN:H	2.22	0.47
1:P:106:LEU:HD13	1:P:106:LEU:O	2.14	0.47
1:F:78:LEU:HD21	1:F:297:ILE:HG22	1.97	0.47
1:F:271:ILE:HG12	1:F:272:ILE:N	2.29	0.47
1:I:101:ASN:HD22	1:I:104:LYS:H	1.62	0.47
1:P:116:GLN:HE21	1:P:116:GLN:HB3	1.55	0.47
1:P:166:PHE:CE2	1:P:203:ALA:HA	2.49	0.47
1:F:90:LYS:HB2	1:F:90:LYS:NZ	2.30	0.47
1:D:117:VAL:O	1:D:140:VAL:HG11	2.16	0.46
1:A:86:ALA:CB	1:A:93:ILE:HD11	2.45	0.46
1:D:274:PHE:O	1:D:275:ASP:CB	2.64	0.46
1:B:70:ILE:HG22	1:B:97:ASN:ND2	2.30	0.46
1:I:157:VAL:CG1	1:I:301:ALA:HB2	2.46	0.46
1:P:79:ALA:O	1:P:82:ILE:HB	2.15	0.46
1:F:173:ILE:HD12	1:F:209:LEU:CD1	2.45	0.46
1:A:94:ILE:HD11	1:D:115:LYS:HZ3	1.81	0.46
1:D:191:ILE:O	1:D:195:LYS:HB2	2.15	0.46
1:B:244:PHE:HD1	1:B:272:ILE:HG23	1.80	0.46
1:B:303:ARG:HH21	2:B:5256:171:HN	1.63	0.46
1:P:186:THR:HG22	1:P:188:GLU:H	1.81	0.46
1:F:215:TYR:C	1:F:216:ILE:HD12	2.40	0.46
1:A:146:ALA:CA	1:A:158:THR:HG22	2.46	0.46
1:A:173:ILE:HD13	1:A:180:ILE:CD1	2.46	0.46
1:A:201:LYS:O	1:A:205:THR:HG23	2.15	0.46
1:A:282:MET:HG2	1:D:223:TYR:CG	2.50	0.46
1:D:219:GLY:HA3	1:D:250:MET:CE	2.45	0.46
1:B:288:THR:HG23	1:B:330:SER:OG	2.16	0.46
1:I:90:LYS:HD3	1:I:90:LYS:C	2.41	0.46
1:P:67:ILE:HG22	1:P:123:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:VAL:HA	1:D:121:ILE:O	2.16	0.46
1:I:101:ASN:HD21	1:I:103:ASP:HB2	1.80	0.46
1:F:223:TYR:CE2	1:F:227:ILE:HD11	2.51	0.46
1:F:261:ARG:HB3	1:F:261:ARG:HH11	1.80	0.46
1:A:173:ILE:HD12	1:A:209:LEU:CD1	2.45	0.46
1:A:233:LEU:O	1:A:236:GLU:HB2	2.16	0.46
1:A:236:GLU:O	1:A:237:ASP:C	2.58	0.46
1:A:314:VAL:HG11	1:A:317:SER:HA	1.98	0.46
1:P:129:GLU:HA	1:P:132:VAL:CG1	2.46	0.46
1:F:73:ILE:H	1:F:73:ILE:CD1	2.29	0.46
1:D:169:VAL:HG23	1:D:180:ILE:HG21	1.98	0.46
1:I:121:ILE:HD12	1:I:305:LEU:HD22	1.98	0.46
1:P:122:PHE:O	1:P:144:LEU:HA	2.16	0.46
1:P:280:SER:HB3	1:P:328:ARG:NH1	2.30	0.46
1:F:66:ILE:HB	1:F:122:PHE:HD2	1.80	0.46
1:D:93:ILE:C	1:D:94:ILE:HD12	2.41	0.46
1:B:184:SER:OG	1:B:185:GLY:N	2.48	0.46
1:I:61:THR:HB	1:I:91:TYR:CD1	2.51	0.46
1:F:327:PHE:HD2	1:F:331:THR:HG21	1.81	0.46
1:A:77:GLU:HB3	1:A:294:MET:CE	2.41	0.46
1:I:72:ASN:ND2	1:I:74:PHE:H	2.14	0.46
1:F:151:THR:CG2	1:F:153:GLN:HG2	2.44	0.46
1:D:189:GLU:HA	1:D:190:PRO:HD3	1.86	0.46
1:B:73:ILE:HD13	1:B:73:ILE:N	2.19	0.46
1:I:177:HIS:ND1	1:I:241:THR:HB	2.30	0.46
1:I:252:LEU:HG	1:I:283:VAL:HG13	1.96	0.46
1:P:307:LYS:CE	1:P:314:VAL:HG21	2.46	0.46
1:A:153:GLN:HB3	3:A:541:HOH:O	2.17	0.45
1:D:220:ASP:O	1:D:221:TYR:HB2	2.16	0.45
1:I:79:ALA:HB1	1:I:95:LEU:HD21	1.98	0.45
1:F:98:SER:O	1:F:99:ASP:HB2	2.15	0.45
1:F:182:PHE:HB2	1:F:200:TYR:CE2	2.50	0.45
1:A:94:ILE:HG23	1:D:94:ILE:HG23	1.98	0.45
1:A:305:LEU:CG	1:A:309:MET:HE2	2.27	0.45
1:I:242:ALA:HA	1:I:270:GLU:O	2.16	0.45
1:B:123:MET:HG2	1:B:145:ALA:HB3	1.99	0.45
1:I:179:ASN:HB3	1:I:215:TYR:OH	2.15	0.45
1:D:68:PRO:HB3	1:D:100:GLN:HG3	1.99	0.45
1:D:318:ILE:O	1:D:318:ILE:HD13	2.16	0.45
1:B:189:GLU:HB2	1:B:192:ASN:HD22	1.80	0.45
1:F:287:LEU:HD12	1:F:288:THR:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:MET:O	1:D:254:VAL:HG23	2.16	0.45
1:B:178:LYS:HA	1:B:209:LEU:HD13	1.97	0.45
1:B:319:VAL:HG12	1:B:320:GLN:H	1.81	0.45
1:D:266:PRO:HD3	1:D:329:GLN:O	2.16	0.45
1:B:220:ASP:O	1:B:221:TYR:HB2	2.17	0.45
1:F:83:GLU:O	1:F:87:THR:HG23	2.16	0.45
1:A:136:LYS:HE3	1:A:153:GLN:HE21	1.81	0.45
1:B:134:GLU:O	1:B:137:LYS:HG2	2.17	0.45
1:F:190:PRO:O	1:F:194:ALA:HB3	2.16	0.45
1:F:219:GLY:HA3	1:F:250:MET:CE	2.44	0.45
1:D:287:LEU:HA	1:D:330:SER:HB2	1.99	0.45
1:B:230:VAL:CG2	1:B:257:GLY:HA3	2.44	0.45
1:B:252:LEU:HG	1:B:283:VAL:HG11	1.96	0.45
1:D:292:GLN:O	1:D:292:GLN:HG3	2.17	0.45
1:B:135:LEU:HD23	1:B:136:LYS:N	2.31	0.45
1:P:132:VAL:HG23	1:P:154:ILE:CG1	2.47	0.45
1:A:113:LEU:HD21	1:A:140:VAL:HG22	1.99	0.44
1:A:175:SER:HB2	1:A:177:HIS:HD2	1.81	0.44
1:A:179:ASN:HB3	1:A:212:ARG:HH21	1.81	0.44
1:D:219:GLY:HA3	1:D:250:MET:HE1	1.99	0.44
1:P:112:MET:O	1:P:117:VAL:HG13	2.17	0.44
1:P:303:ARG:O	1:P:307:LYS:HG3	2.17	0.44
1:F:72:ASN:ND2	1:F:72:ASN:C	2.74	0.44
1:D:108:LEU:O	1:D:112:MET:HG2	2.16	0.44
1:D:144:LEU:HB2	1:D:156:SER:HB3	1.99	0.44
1:B:135:LEU:HD23	1:B:135:LEU:C	2.41	0.44
1:F:307:LYS:O	1:F:312:GLU:HB2	2.17	0.44
1:B:255:ILE:HG22	1:B:259:GLN:OE1	2.17	0.44
1:P:187:LEU:HB2	1:P:218:GLU:OE2	2.18	0.44
1:P:108:LEU:O	1:P:112:MET:HG2	2.17	0.44
1:P:271:ILE:C	1:P:272:ILE:HD12	2.42	0.44
1:P:317:SER:HB3	1:P:318:ILE:HD12	2.00	0.44
1:F:123:MET:CG	1:F:145:ALA:HB3	2.47	0.44
1:F:305:LEU:HG	1:F:309:MET:HG3	2.00	0.44
1:B:78:LEU:HD13	1:B:123:MET:SD	2.57	0.44
1:I:190:PRO:HA	1:I:193:HIS:CE1	2.51	0.44
1:F:94:ILE:CG2	1:F:112:MET:HE1	2.48	0.44
1:B:70:ILE:HG22	1:B:97:ASN:HD21	1.81	0.44
1:B:185:GLY:O	1:B:186:THR:C	2.60	0.44
1:B:264:ASN:OD1	1:B:267:ASN:HB2	2.17	0.44
1:I:269:LEU:HD13	1:I:271:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ILE:HG21	1:D:112:MET:HE1	1.99	0.44
1:D:169:VAL:HG13	1:D:203:ALA:CB	2.48	0.44
1:P:162:GLU:OE2	1:P:202:ARG:NH1	2.50	0.44
1:F:91:TYR:CE1	1:F:309:MET:CE	3.01	0.44
1:F:226:GLY:O	1:F:254:VAL:HG22	2.18	0.44
1:B:305:LEU:O	1:B:309:MET:HG3	2.18	0.44
1:I:185:GLY:HA3	1:I:221:TYR:CE2	2.53	0.44
1:I:245:VAL:HG11	1:I:251:ALA:N	2.32	0.44
1:A:217:VAL:HG21	1:A:229:ALA:HB1	2.00	0.44
1:B:284:ARG:HH11	1:I:256:HIS:HB3	1.82	0.44
1:P:183:VAL:HB	1:P:245:VAL:HG22	2.00	0.44
1:F:264:ASN:OD1	1:F:267:ASN:HB2	2.18	0.44
1:B:159:ILE:CG1	1:B:323:HIS:HB3	2.47	0.43
1:B:193:HIS:ND1	1:B:194:ALA:N	2.65	0.43
1:F:287:LEU:HA	1:F:330:SER:HB3	2.00	0.43
1:F:325:ILE:N	1:F:325:ILE:HD12	2.33	0.43
1:D:271:ILE:O	1:D:330:SER:OG	2.32	0.43
1:P:84:ASP:O	1:P:88:MET:HE3	2.19	0.43
1:F:212:ARG:HH12	1:F:238:GLU:HB2	1.83	0.43
1:F:284:ARG:HA	1:F:285:PRO:C	2.43	0.43
1:D:223:TYR:CE1	1:D:253:GLY:HA2	2.53	0.43
1:B:109:LEU:O	1:B:113:LEU:HG	2.18	0.43
1:I:220:ASP:OD2	1:I:225:SER:HB3	2.18	0.43
1:A:101:ASN:OD1	1:A:101:ASN:O	2.37	0.43
1:A:128:THR:O	1:A:131:HIS:HB2	2.17	0.43
1:A:212:ARG:HD2	1:A:215:TYR:CD1	2.53	0.43
1:I:158:THR:OG1	1:I:159:ILE:N	2.51	0.43
1:P:284:ARG:HG2	1:P:284:ARG:HH11	1.83	0.43
1:A:101:ASN:OD1	1:A:103:ASP:HB2	2.18	0.43
1:D:204:LEU:HD12	1:D:209:LEU:HD12	1.99	0.43
1:I:89:TYR:O	1:I:90:LYS:CG	2.66	0.43
1:P:306:THR:HA	1:P:309:MET:CE	2.48	0.43
1:F:243:ILE:HG13	1:F:269:LEU:HD21	1.99	0.43
1:A:255:ILE:O	1:A:259:GLN:HG3	2.18	0.43
1:D:144:LEU:HG	1:D:154:ILE:CG2	2.49	0.43
1:B:174:ASP:OD1	1:B:174:ASP:N	2.51	0.43
1:B:286:GLN:O	1:B:328:ARG:HB2	2.19	0.43
1:B:310:ASN:O	1:B:311:LYS:HB2	2.17	0.43
1:F:163:GLN:O	1:F:166:PHE:HB3	2.19	0.43
1:F:181:ALA:HA	1:F:215:TYR:HB3	2.00	0.43
1:A:187:LEU:O	1:A:193:HIS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:THR:CB	1:D:286:GLN:HE21	2.32	0.43
1:B:66:ILE:HG13	1:B:122:PHE:HD2	1.84	0.43
1:B:276:ASN:HB2	1:B:291:VAL:HA	1.99	0.43
1:I:72:ASN:ND2	1:I:73:ILE:N	2.64	0.43
1:I:241:THR:O	1:I:269:LEU:HD23	2.19	0.43
1:D:131:HIS:O	1:D:135:LEU:HB2	2.18	0.43
1:B:148:ILE:CG1	1:B:191:ILE:HG13	2.48	0.43
1:P:94:ILE:HD11	1:F:94:ILE:CD1	2.40	0.43
1:A:164:ALA:HB1	1:A:290:VAL:HG11	2.01	0.43
1:I:166:PHE:CD1	1:I:166:PHE:C	2.96	0.43
1:F:232:LYS:O	1:F:235:GLU:HB2	2.19	0.43
1:A:117:VAL:O	1:A:140:VAL:HG11	2.18	0.42
1:D:106:LEU:HD22	1:D:110:ASN:ND2	2.34	0.42
1:D:223:TYR:OH	1:D:256:HIS:CD2	2.69	0.42
1:F:190:PRO:HA	1:F:193:HIS:NE2	2.33	0.42
1:F:270:GLU:HB2	1:F:331:THR:HA	2.01	0.42
1:A:166:PHE:CD1	1:A:166:PHE:C	2.98	0.42
1:A:179:ASN:HB2	1:A:215:TYR:CE2	2.54	0.42
1:D:121:ILE:CD1	1:D:302:MET:HG2	2.49	0.42
1:B:178:LYS:C	1:B:178:LYS:HD3	2.44	0.42
1:B:201:LYS:O	1:B:202:ARG:C	2.63	0.42
1:I:138:SER:HA	1:I:139:PRO:HD3	1.84	0.42
1:P:94:ILE:C	1:P:94:ILE:HD13	2.44	0.42
1:P:222:THR:HG22	1:P:224:ASP:H	1.84	0.42
1:A:193:HIS:CD2	1:A:193:HIS:C	2.97	0.42
1:B:159:ILE:HG23	1:B:161:TYR:CE2	2.55	0.42
1:P:67:ILE:HG22	1:P:123:MET:CE	2.49	0.42
1:P:182:PHE:HD2	1:P:244:PHE:CD2	2.36	0.42
1:P:266:PRO:HB3	1:P:330:SER:O	2.19	0.42
1:F:255:ILE:HD11	1:F:271:ILE:HD12	2.02	0.42
1:B:97:ASN:O	1:B:108:LEU:HD11	2.20	0.42
1:I:117:VAL:O	1:I:140:VAL:HG11	2.20	0.42
1:P:151:THR:O	1:P:151:THR:HG22	2.19	0.42
1:P:241:THR:O	1:P:269:LEU:HA	2.20	0.42
1:A:169:VAL:O	1:A:173:ILE:HG12	2.20	0.42
1:B:222:THR:CG2	1:B:224:ASP:H	2.33	0.42
1:B:319:VAL:CG1	1:B:320:GLN:N	2.82	0.42
1:P:282:MET:HG2	1:F:223:TYR:CG	2.55	0.42
1:F:197:VAL:CG1	1:F:198:LYS:N	2.82	0.42
1:B:159:ILE:HG12	1:B:160:ASP:H	1.85	0.42
1:B:245:VAL:HG12	1:B:247:THR:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:VAL:HG12	1:B:271:ILE:HG12	2.01	0.42
1:I:111:ASN:CG	1:I:115:LYS:HZ2	2.27	0.42
1:I:190:PRO:O	1:I:194:ALA:HB3	2.20	0.42
1:F:73:ILE:N	1:F:73:ILE:CD1	2.83	0.42
1:F:123:MET:HG2	1:F:145:ALA:HB3	2.01	0.42
1:F:193:HIS:CD2	1:F:193:HIS:C	2.97	0.42
1:F:267:ASN:OD1	1:F:332:LYS:HE3	2.20	0.42
1:B:63:VAL:HG22	1:B:93:ILE:CD1	2.50	0.42
1:B:315:ASP:O	1:B:316:SER:HB2	2.19	0.42
1:I:61:THR:H	1:I:90:LYS:NZ	2.17	0.42
1:P:145:ALA:O	1:P:146:ALA:C	2.62	0.42
1:P:267:ASN:HD22	1:P:332:LYS:CE	2.33	0.42
1:F:220:ASP:O	1:F:221:TYR:HB2	2.20	0.42
1:F:252:LEU:HG	1:F:283:VAL:HG13	2.01	0.42
1:F:264:ASN:O	1:F:268:ASP:HB2	2.19	0.42
1:A:227:ILE:O	1:A:230:VAL:HG23	2.20	0.42
1:D:182:PHE:CZ	1:D:184:SER:HB2	2.54	0.42
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.84	0.42
1:F:95:LEU:C	1:F:95:LEU:HD23	2.45	0.42
1:A:148:ILE:HD12	1:A:190:PRO:HB3	2.02	0.42
1:D:82:ILE:HG23	1:D:121:ILE:HD12	2.00	0.42
1:B:168:ALA:O	1:B:171:SER:HB3	2.19	0.42
1:B:303:ARG:HE	1:B:303:ARG:HB2	1.65	0.42
1:P:248:ASP:OD1	1:P:277:THR:HG22	2.19	0.42
1:F:166:PHE:CD1	1:F:166:PHE:C	2.98	0.42
1:A:148:ILE:HD12	1:A:190:PRO:HB2	2.02	0.41
1:D:191:ILE:HD11	1:D:196:LYS:HE3	2.02	0.41
1:B:122:PHE:CZ	1:B:124:SER:HB2	2.55	0.41
1:I:112:MET:HA	1:I:115:LYS:CD	2.49	0.41
1:I:202:ARG:O	1:I:206:GLU:HG3	2.19	0.41
1:P:277:THR:HG23	1:P:278:ARG:N	2.34	0.41
1:A:321:LEU:HD23	1:A:322:PRO:HD2	2.01	0.41
1:B:321:LEU:HD13	1:B:322:PRO:HD2	2.01	0.41
1:I:114:GLY:C	1:I:116:GLN:N	2.75	0.41
1:P:154:ILE:HD13	1:P:154:ILE:HA	1.93	0.41
1:P:295:TYR:HB3	3:P:593:HOH:O	2.20	0.41
1:A:101:ASN:OD1	1:A:101:ASN:C	2.63	0.41
1:D:64:GLY:O	1:D:120:ILE:HA	2.20	0.41
1:D:246:GLY:O	1:D:274:PHE:HB3	2.20	0.41
1:P:105:GLU:O	1:P:109:LEU:HB2	2.20	0.41
1:P:120:ILE:O	1:P:142:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ASP:OD1	1:A:315:ASP:N	2.50	0.41
1:D:212:ARG:HB3	1:D:215:TYR:HB2	2.03	0.41
1:B:109:LEU:C	1:B:109:LEU:HD23	2.45	0.41
1:B:263:LEU:HD13	1:B:269:LEU:HD22	2.03	0.41
1:F:304:LEU:HD11	1:F:314:VAL:HG11	2.01	0.41
1:F:324:ARG:HG2	1:F:325:ILE:H	1.85	0.41
1:D:257:GLY:O	1:D:261:ARG:HG2	2.20	0.41
1:B:209:LEU:HA	1:B:210:PRO:HD3	1.84	0.41
1:B:277:THR:HG22	1:B:279:LEU:HB2	2.03	0.41
1:F:260:ASP:C	1:F:262:GLY:N	2.76	0.41
1:A:148:ILE:HG13	1:A:195:LYS:CE	2.51	0.41
1:D:157:VAL:HB	1:D:319:VAL:HB	2.01	0.41
1:B:285:PRO:HB2	1:B:329:GLN:HB2	2.03	0.41
1:F:169:VAL:O	1:F:173:ILE:HG12	2.21	0.41
1:F:173:ILE:HG21	1:F:207:SER:OG	2.20	0.41
1:D:149:GLU:O	1:D:149:GLU:HG3	2.19	0.41
1:D:267:ASN:HA	1:D:332:LYS:HZ3	1.84	0.41
1:B:241:THR:O	1:B:269:LEU:HA	2.21	0.41
1:F:61:THR:HB	1:F:118:ASP:OD1	2.21	0.41
1:D:89:TYR:O	1:D:90:LYS:HB2	2.19	0.41
1:I:161:TYR:CD1	1:I:191:ILE:HD13	2.56	0.41
1:I:188:GLU:H	1:I:188:GLU:CD	2.29	0.41
1:I:230:VAL:HG22	1:I:254:VAL:HG13	2.01	0.41
1:F:189:GLU:HA	1:F:190:PRO:HD2	1.79	0.41
1:A:66:ILE:HG21	1:A:108:LEU:HD13	2.03	0.41
1:A:115:LYS:HA	1:A:115:LYS:HD3	1.85	0.41
1:A:304:LEU:O	1:A:308:TYR:CD2	2.73	0.41
1:B:99:ASP:CG	1:I:80:ARG:NH2	2.79	0.41
1:B:272:ILE:HG23	1:B:272:ILE:O	2.20	0.41
1:I:80:ARG:HD2	1:I:80:ARG:HA	1.90	0.41
1:P:247:THR:HB	1:P:250:MET:HE2	2.02	0.41
1:P:269:LEU:HG	1:P:271:ILE:HD11	2.02	0.41
1:P:305:LEU:O	1:P:309:MET:HG3	2.20	0.41
1:P:306:THR:HA	1:P:309:MET:HE2	2.03	0.41
1:F:113:LEU:HD22	1:F:139:PRO:HG2	2.03	0.41
1:F:129:GLU:CD	1:F:130:GLU:N	2.78	0.41
1:A:151:THR:O	1:A:152:ASN:HB2	2.20	0.41
1:D:261:ARG:HG3	1:D:261:ARG:NH1	2.35	0.41
1:B:66:ILE:HG13	1:B:66:ILE:O	2.21	0.41
1:B:66:ILE:CG1	1:B:122:PHE:HD2	2.34	0.41
1:B:248:ASP:OD1	1:B:280:SER:OG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:LEU:HD23	1:I:113:LEU:N	2.34	0.41
1:P:72:ASN:HD22	1:P:74:PHE:H	1.67	0.41
1:P:307:LYS:HE3	1:P:314:VAL:HG21	2.02	0.41
1:F:118:ASP:CB	1:F:309:MET:SD	3.09	0.41
1:F:179:ASN:HB3	1:F:215:TYR:CE2	2.55	0.41
1:A:113:LEU:O	1:A:116:GLN:N	2.51	0.40
1:D:68:PRO:CB	1:D:100:GLN:HG3	2.51	0.40
1:D:98:SER:O	1:D:99:ASP:HB2	2.21	0.40
1:D:151:THR:CB	1:D:153:GLN:HE21	2.34	0.40
1:D:231:GLU:HG2	1:D:261:ARG:NH1	2.36	0.40
1:B:239:LYS:HA	1:B:240:PRO:HD3	1.92	0.40
1:B:300:VAL:HG21	1:B:321:LEU:HD21	2.03	0.40
1:F:216:ILE:HD12	1:F:216:ILE:N	2.36	0.40
1:F:271:ILE:HD13	1:F:271:ILE:O	2.21	0.40
1:F:293:PRO:HB2	1:F:296:ASP:HB2	2.03	0.40
1:B:191:ILE:HD11	3:B:586:HOH:O	2.21	0.40
1:B:198:LYS:HZ2	1:B:202:ARG:HD3	1.86	0.40
1:I:230:VAL:HG11	1:I:258:ALA:HB2	2.04	0.40
1:P:115:LYS:O	1:P:116:GLN:C	2.64	0.40
1:P:200:TYR:HE1	1:P:216:ILE:HD11	1.86	0.40
1:A:112:MET:CE	1:A:117:VAL:HG11	2.48	0.40
1:B:148:ILE:HD11	1:B:190:PRO:HB2	2.04	0.40
1:I:98:SER:HA	1:I:104:LYS:HE2	2.02	0.40
1:I:109:LEU:CD2	1:I:135:LEU:HD12	2.51	0.40
1:I:121:ILE:HD12	1:I:121:ILE:N	2.36	0.40
1:I:212:ARG:O	1:I:215:TYR:HB2	2.21	0.40
1:P:238:GLU:OE1	1:P:238:GLU:HA	2.21	0.40
1:A:169:VAL:HG21	1:A:200:TYR:HD2	1.86	0.40
1:B:65:VAL:O	1:B:95:LEU:HA	2.21	0.40
1:I:111:ASN:HD21	1:I:115:LYS:NZ	2.19	0.40
1:P:80:ARG:O	1:P:83:GLU:HB2	2.22	0.40
1:P:128:THR:O	1:P:131:HIS:HB2	2.22	0.40
1:F:132:VAL:HA	1:F:154:ILE:HD11	2.02	0.40
1:F:255:ILE:O	1:F:259:GLN:HG3	2.21	0.40
1:D:152:ASN:HB3	1:D:318:ILE:HG21	2.04	0.40
1:B:189:GLU:HA	1:B:190:PRO:HD3	1.83	0.40
1:B:256:HIS:HD2	1:B:259:GLN:OE1	2.04	0.40
1:B:267:ASN:HA	1:B:332:LYS:HZ3	1.87	0.40
1:I:102:GLN:O	1:I:106:LEU:HB2	2.22	0.40
1:I:166:PHE:CE2	1:I:202:ARG:NH1	2.88	0.40
1:P:72:ASN:HD22	1:P:73:ILE:N	2.18	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	273/280 (98%)	248 (91%)	18 (7%)	7 (3%)	4	7
1	B	271/280 (97%)	230 (85%)	35 (13%)	6 (2%)	5	10
1	D	271/280 (97%)	250 (92%)	17 (6%)	4 (2%)	8	15
1	F	271/280 (97%)	247 (91%)	22 (8%)	2 (1%)	18	34
1	I	273/280 (98%)	248 (91%)	20 (7%)	5 (2%)	6	13
1	P	271/280 (97%)	242 (89%)	23 (8%)	6 (2%)	5	10
All	All	1630/1680 (97%)	1465 (90%)	135 (8%)	30 (2%)	6	13

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	150	SER
1	B	150	SER
1	B	316	SER
1	P	68	PRO
1	P	313	THR
1	F	275	ASP
1	A	71	SER
1	A	237	ASP
1	A	275	ASP
1	D	275	ASP
1	B	275	ASP
1	I	275	ASP
1	I	316	SER
1	P	275	ASP
1	D	186	THR
1	B	267	ASN

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Mol	Chain	Res	Type
1	I	116	GLN
1	I	139	PRO
1	P	150	SER
1	A	293	PRO
1	P	141	PRO
1	D	293	PRO
1	B	203	ALA
1	I	115	LYS
1	A	139	PRO
1	P	132	VAL
1	F	293	PRO
1	D	211	VAL
1	B	68	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	241/244 (99%)	218 (90%)	23 (10%)	8	16
1	B	239/244 (98%)	211 (88%)	28 (12%)	5	9
1	D	239/244 (98%)	216 (90%)	23 (10%)	8	15
1	F	239/244 (98%)	211 (88%)	28 (12%)	5	9
1	I	241/244 (99%)	206 (86%)	35 (14%)	3	5
1	P	239/244 (98%)	205 (86%)	34 (14%)	3	6
All	All	1438/1464 (98%)	1267 (88%)	171 (12%)	5	8

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	VAL
1	A	66	ILE
1	A	73	ILE
1	A	78	LEU
1	A	80	ARG

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Mol	Chain	Res	Type
1	A	84	ASP
1	A	95	LEU
1	A	96	SER
1	A	100	GLN
1	A	101	ASN
1	A	115	LYS
1	A	133	GLU
1	A	142	VAL
1	A	143	VAL
1	A	148	ILE
1	A	157	VAL
1	A	162	GLU
1	A	163	GLN
1	A	180	ILE
1	A	216	ILE
1	A	230	VAL
1	A	288	THR
1	A	319	VAL
1	D	60	THR
1	D	61	THR
1	D	62	THR
1	D	63	VAL
1	D	65	VAL
1	D	87	THR
1	D	95	LEU
1	D	96	SER
1	D	106	LEU
1	D	109	LEU
1	D	129	GLU
1	D	148	ILE
1	D	149	GLU
1	D	157	VAL
1	D	188	GLU
1	D	198	LYS
1	D	204	LEU
1	D	241	THR
1	D	269	LEU
1	D	283	VAL
1	D	292	GLN
1	D	302	MET
1	D	318	ILE
1	B	63	VAL

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Mol	Chain	Res	Type
1	B	65	VAL
1	B	67	ILE
1	B	73	ILE
1	B	93	ILE
1	B	95	LEU
1	B	112	MET
1	B	120	ILE
1	B	133	GLU
1	B	135	LEU
1	B	143	VAL
1	B	148	ILE
1	B	157	VAL
1	B	159	ILE
1	B	162	GLU
1	B	179	ASN
1	B	191	ILE
1	B	205	THR
1	B	212	ARG
1	B	222	THR
1	B	236	GLU
1	B	266	PRO
1	B	268	ASP
1	B	277	THR
1	B	283	VAL
1	B	284	ARG
1	B	303	ARG
1	B	310	ASN
1	I	62	THR
1	I	63	VAL
1	I	67	ILE
1	I	71	SER
1	I	77	GLU
1	I	78	LEU
1	I	90	LYS
1	I	93	ILE
1	I	95	LEU
1	I	97	ASN
1	I	106	LEU
1	I	111	ASN
1	I	112	MET
1	I	113	LEU
1	I	132	VAL

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Mol	Chain	Res	Type
1	I	135	LEU
1	I	143	VAL
1	I	147	SER
1	I	149	GLU
1	I	157	VAL
1	I	169	VAL
1	I	188	GLU
1	I	198	LYS
1	I	212	ARG
1	I	237	ASP
1	I	241	THR
1	I	247	THR
1	I	269	LEU
1	I	271	ILE
1	I	283	VAL
1	I	302	MET
1	I	304	LEU
1	I	313	THR
1	I	318	ILE
1	I	324	ARG
1	P	60	THR
1	P	62	THR
1	P	65	VAL
1	P	70	ILE
1	P	72	ASN
1	P	73	ILE
1	P	85	ILE
1	P	92	ASN
1	P	93	ILE
1	P	94	ILE
1	P	111	ASN
1	P	113	LEU
1	P	116	GLN
1	P	129	GLU
1	P	142	VAL
1	P	143	VAL
1	P	148	ILE
1	P	149	GLU
1	P	157	VAL
1	P	158	THR
1	P	162	GLU
1	P	163	GLN

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Mol	Chain	Res	Type
1	P	212	ARG
1	P	217	VAL
1	P	230	VAL
1	P	236	GLU
1	P	247	THR
1	P	266	PRO
1	P	277	THR
1	P	283	VAL
1	P	284	ARG
1	P	288	THR
1	P	297	ILE
1	P	303	ARG
1	F	63	VAL
1	F	67	ILE
1	F	72	ASN
1	F	73	ILE
1	F	78	LEU
1	F	83	GLU
1	F	90	LYS
1	F	101	ASN
1	F	106	LEU
1	F	121	ILE
1	F	135	LEU
1	F	149	GLU
1	F	159	ILE
1	F	169	VAL
1	F	180	ILE
1	F	204	LEU
1	F	230	VAL
1	F	247	THR
1	F	261	ARG
1	F	264	ASN
1	F	266	PRO
1	F	269	LEU
1	F	271	ILE
1	F	283	VAL
1	F	294	MET
1	F	309	MET
1	F	318	ILE
1	F	331	THR

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	102	GLN
1	A	107	HIS
1	A	126	ASN
1	A	152	ASN
1	A	153	GLN
1	A	179	ASN
1	A	193	HIS
1	A	310	ASN
1	D	72	ASN
1	D	100	GLN
1	D	110	ASN
1	D	126	ASN
1	D	153	GLN
1	D	163	GLN
1	D	170	GLN
1	D	179	ASN
1	D	192	ASN
1	D	193	HIS
1	D	256	HIS
1	D	286	GLN
1	D	310	ASN
1	B	97	ASN
1	B	101	ASN
1	B	110	ASN
1	B	111	ASN
1	B	126	ASN
1	B	152	ASN
1	B	163	GLN
1	B	177	HIS
1	B	179	ASN
1	B	192	ASN
1	B	292	GLN
1	I	72	ASN
1	I	92	ASN
1	I	101	ASN
1	I	102	GLN
1	I	107	HIS
1	I	110	ASN
1	I	116	GLN
1	I	131	HIS
1	I	153	GLN
1	I	163	GLN
1	I	192	ASN

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Mol	Chain	Res	Type
1	I	286	GLN
1	I	310	ASN
1	P	72	ASN
1	P	100	GLN
1	P	102	GLN
1	P	111	ASN
1	P	116	GLN
1	P	152	ASN
1	P	192	ASN
1	P	267	ASN
1	P	286	GLN
1	P	329	GLN
1	F	72	ASN
1	F	97	ASN
1	F	100	GLN
1	F	101	ASN
1	F	102	GLN
1	F	163	GLN
1	F	193	HIS
1	F	329	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](#)

2 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
2	171	A	3256	-	13,13,13	1.97	4 (30%)	16,17,17	2.15	4 (25%)
2	171	B	5256	-	13,13,13	2.26	5 (38%)	16,17,17	2.33	3 (18%)

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
2	171	A	3256	-	-	2/7/7/7	0/1/1/1
2	171	B	5256	-	-	2/7/7/7	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5256	171	C2-S	-5.63	1.69	1.77
2	A	3256	171	O2-S	3.94	1.56	1.45
2	A	3256	171	O1-S	2.88	1.53	1.45
2	B	5256	171	C3'-C2'	2.85	1.43	1.38
2	A	3256	171	C2-S	-2.46	1.74	1.77
2	A	3256	171	C6'-C1'	2.28	1.43	1.39
2	B	5256	171	C6'-C1'	2.26	1.43	1.39
2	B	5256	171	C5'-C6'	2.09	1.42	1.38
2	B	5256	171	C4'-C3'	2.02	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5256	171	C1-N-C1'	-6.91	107.64	122.92
2	A	3256	171	C1-N-C1'	-6.04	109.56	122.92
2	B	5256	171	C2-C1-N	4.40	124.39	111.41
2	A	3256	171	C2-C1-N	3.92	122.99	111.41
2	B	5256	171	O1-S-C2	2.63	110.69	106.73
2	A	3256	171	O1-S-C2	2.53	110.55	106.73
2	A	3256	171	O2-S-C2	2.34	110.27	106.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5256	171	C2'-C1'-N-C1
2	A	3256	171	C2'-C1'-N-C1
2	B	5256	171	C6'-C1'-N-C1
2	A	3256	171	C6'-C1'-N-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5256	171	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	275/280 (98%)	-0.20	5 (1%) 67 65	17, 34, 57, 72	0
1	B	273/280 (97%)	0.26	4 (1%) 72 71	30, 48, 65, 73	0
1	D	273/280 (97%)	-0.06	1 (0%) 88 89	22, 39, 59, 70	0
1	F	273/280 (97%)	0.11	6 (2%) 62 60	24, 45, 62, 75	0
1	I	275/280 (98%)	0.12	5 (1%) 67 65	22, 42, 65, 76	0
1	P	273/280 (97%)	0.06	2 (0%) 84 84	19, 43, 73, 79	0
All	All	1642/1680 (97%)	0.05	23 (1%) 73 73	17, 42, 65, 79	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	GLY	5.5
1	I	116	GLN	4.3
1	I	114	GLY	3.8
1	F	316	SER	3.0
1	A	113	LEU	2.9
1	F	315	ASP	2.9
1	F	314	VAL	2.9
1	P	113	LEU	2.6
1	B	315	ASP	2.6
1	I	113	LEU	2.6
1	I	115	LYS	2.4
1	A	115	LYS	2.3
1	F	60	THR	2.3
1	P	313	THR	2.3
1	B	179	ASN	2.3
1	B	151	THR	2.2
1	A	315	ASP	2.2
1	I	107	HIS	2.2
1	B	313	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	234	LEU	2.1
1	D	266	PRO	2.1
1	F	125	GLY	2.1
1	A	116	GLN	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	171	A	3256	13/13	0.79	0.18	20,23,29,40	0
2	171	B	5256	13/13	0.90	0.17	21,23,28,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.