



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:29 PM UTC

PDB ID : 1RYZ / pdb_00001ryz
Title : Uridine Phosphorylase from Salmonella typhimurium. Crystal Structure at 2.9 Å Resolution
Authors : Dontsova, M.V.; Gabdoulkhakov, A.G.; Lyashenko, A.V.; Nikonov, S.V.; Ealick, S.E.; Mikhailov, A.M.
Deposited on : 2003-12-23
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

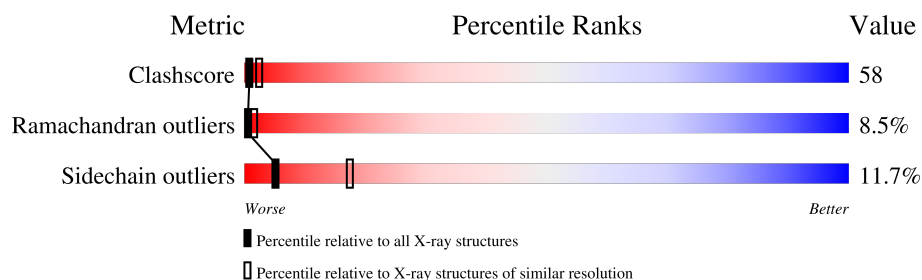
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	253	29% 54% 13% ..
1	B	253	26% 58% 13% ..
1	C	253	27% 56% 15% ..
1	D	253	30% 53% 15% ..
1	E	253	26% 57% 13% ..
1	F	253	26% 54% 16% ..

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACY	B	254	-	-	X	-

2 Entry composition [i](#)

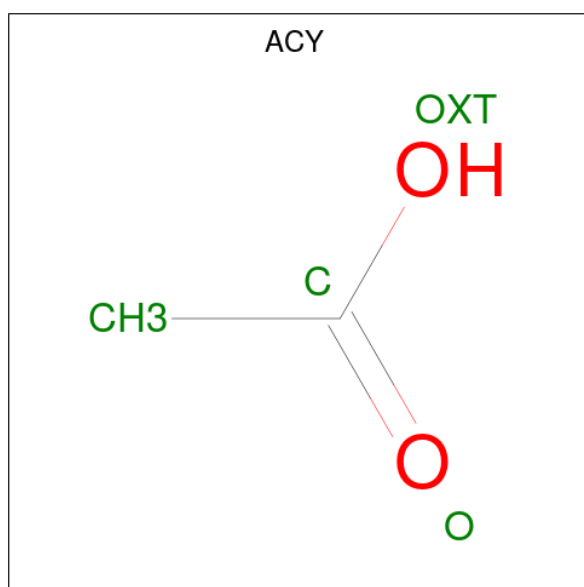
There are 2 unique types of molecules in this entry. The entry contains 11270 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	B	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	C	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	D	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	E	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	F	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			

- Molecule 2 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



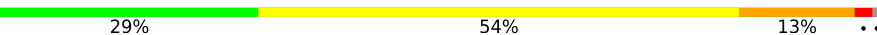
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

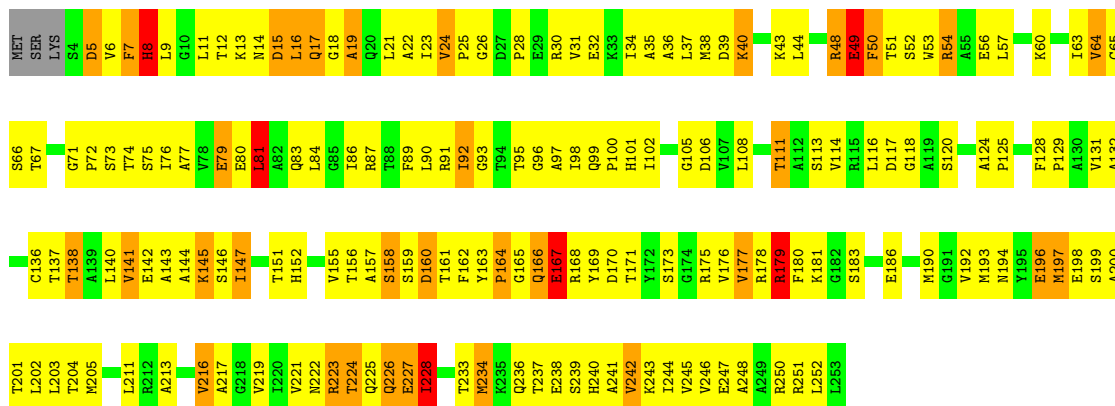
3 Residue-property plots

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

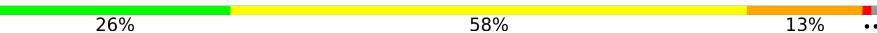
Note EDS was not executed.

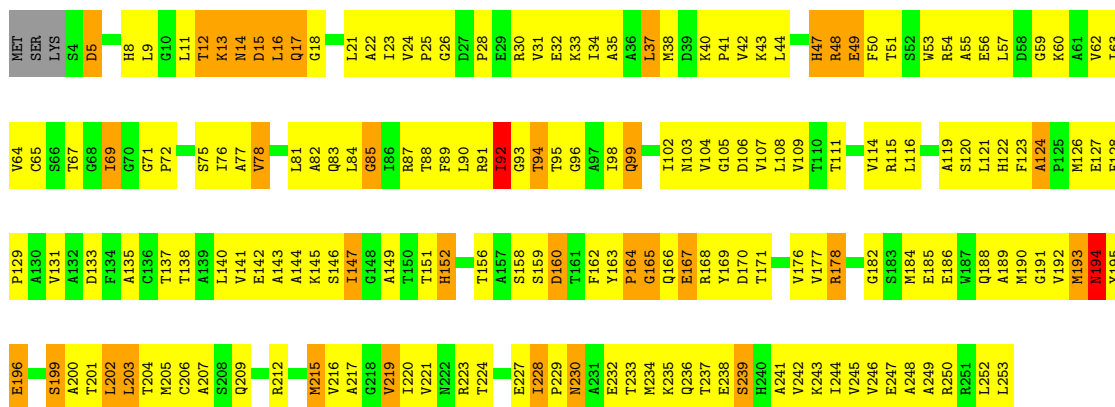
• Molecule 1: Uridine phosphorylase

Chain A: 

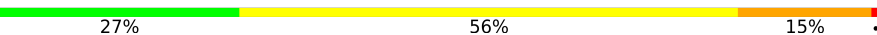


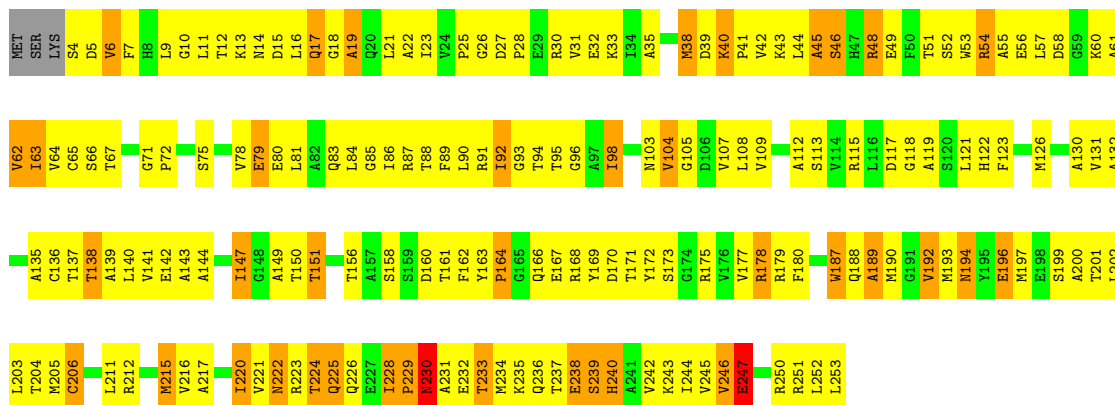
• Molecule 1: Uridine phosphorylase

Chain B: 



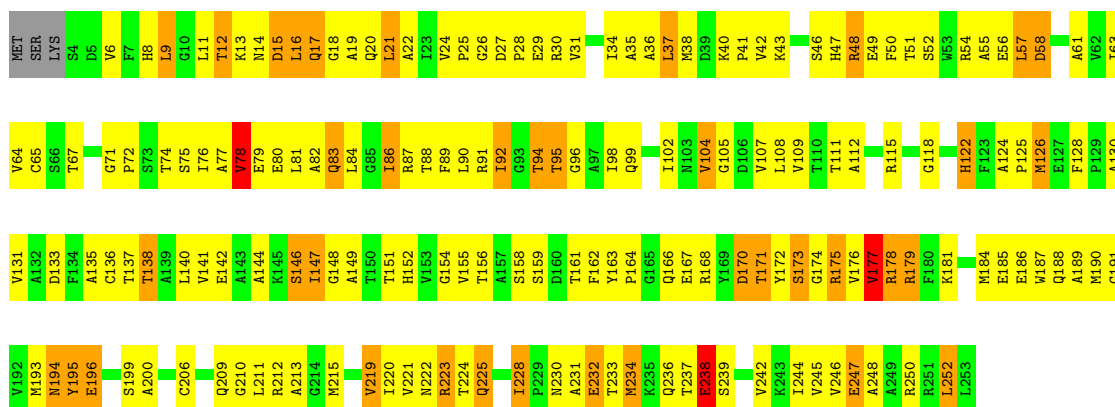
• Molecule 1: Uridine phosphorylase

Chain C: 



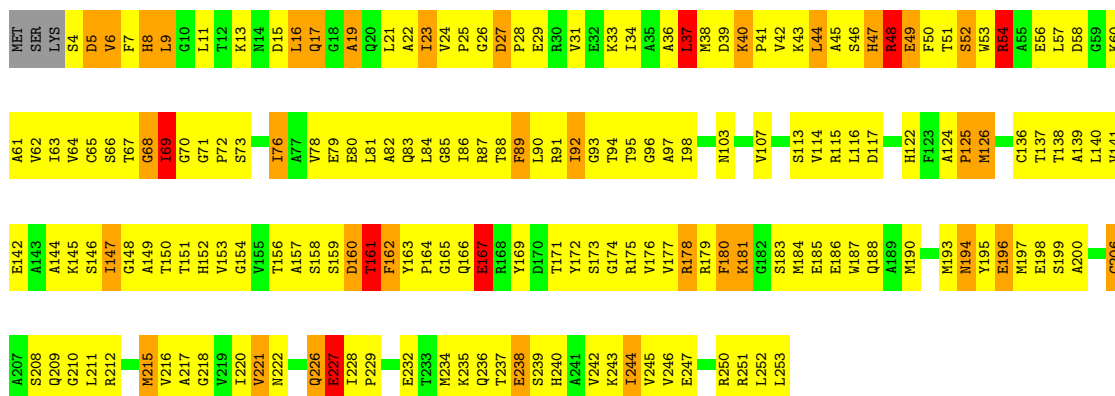
• Molecule 1: Uridine phosphorylase

Chain D: 30% 53% 15% ..



• Molecule 1: Uridine phosphorylase

Chain E: 26% 57% 13% ..



• Molecule 1: Uridine phosphorylase

Chain F: 26% 54% 16% ..

E198	A132	G71	MET
S199	D133	P72	SER
A200	T138		LYS
T201	A139	S75	S4
L202	L140	I76	D5
T204	V141	A77	V6
M205	E142	V78	F7
C206	A143	E79	H8
A207	K144	E80	L9
S208	K145	L81	G10
Q209	S146	A82	L11
	I147	Q83	T12
R212	G148	L84	K13
	A149	G85	M14
M215	T150	I86	D15
V216	T151	R87	L16
A217	H152	T88	Q17
G218	V153	F89	
V219	G154	L90	L21
I220	V155	R91	A22
V221	T156	I92	I23
N222	A157	G93	V24
R223	S158	T94	P25
	S159	T95	G26
	D160	Q96	D27
E227	T161	A97	P28
I228	F162	I98	E29
P229	Y163	Q99	R30
N230	P164	P100	V31
A231	G165	H101	E32
E232	Q166	I102	K33
T233	E167	N103	I34
K235	R168	V104	A35
Q236	Y169	G105	A36
T237	D170	D106	L37
E238	T171	V107	M38
S239	Y172	L108	D39
H240	S173	V109	
A241	G174	T110	L44
V242	R175	T111	
K243	V176	A112	H47
I244	V177	S113	R48
	R178	V114	E49
	R179	R115	F50
E247	F180	D117	T51
A249		G118	S52
R250	M184	A119	W53
L252	E185	S120	R54
L253	E186		A55
	W187	F123	E56
	Q188	A124	L57
		P125	D58
	V192	M126	K60
	M193	E127	A61
	K194	F128	V62
	Y195	P129	I63
	E196	A130	V64
	M197	V131	C65
			S66

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	92.26 Å 92.26 Å 267.46 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.46 – 2.90	Depositor
% Data completeness (in resolution range)	93.9 (29.46-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	0.18	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11270	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.53	0/1907	1.13	16/2584 (0.6%)
1	B	0.51	0/1907	1.07	14/2584 (0.5%)
1	C	0.50	0/1907	1.07	14/2584 (0.5%)
1	D	0.51	0/1907	1.05	10/2584 (0.4%)
1	E	0.54	0/1907	1.11	15/2584 (0.6%)
1	F	0.52	0/1907	1.11	14/2584 (0.5%)
All	All	0.52	0/11442	1.09	83/15504 (0.5%)

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	VAL	N-CA-C	-9.13	94.29	108.44
1	F	98	ILE	N-CA-C	-8.94	104.66	111.90
1	F	227	GLU	N-CA-C	8.64	122.28	109.24
1	E	47	HIS	N-CA-C	7.81	124.98	114.12
1	F	49	GLU	N-CA-C	-7.64	101.63	113.02
1	C	247	GLU	N-CA-C	-7.20	103.43	111.28
1	D	52	SER	N-CA-C	7.18	120.48	108.20
1	F	184	MET	N-CA-C	-7.17	102.27	111.02
1	A	24	VAL	CA-C-N	7.16	128.79	119.84
1	A	24	VAL	C-N-CA	7.16	128.79	119.84
1	F	234	MET	N-CA-C	-7.11	105.04	113.21
1	B	15	ASP	N-CA-C	-6.92	104.66	113.23
1	B	124	ALA	N-CA-C	6.91	114.35	108.13
1	D	252	LEU	N-CA-C	6.89	119.67	111.33
1	E	89	PHE	N-CA-C	6.89	118.89	109.11
1	F	47	HIS	N-CA-C	6.84	121.54	111.34
1	E	23	ILE	N-CA-C	-6.83	98.74	108.58
1	C	194	ASN	N-CA-C	6.71	118.00	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	MET	N-CA-C	-6.64	105.16	113.20
1	A	81	LEU	N-CA-C	-6.63	103.98	111.07
1	F	206	CYS	N-CA-C	6.52	118.08	110.97
1	C	103	ASN	N-CA-C	6.39	119.95	109.85
1	E	161	THR	N-CA-C	6.37	118.07	108.46
1	C	224	THR	N-CA-C	-6.29	104.71	112.38
1	B	152	HIS	N-CA-C	-6.22	99.59	109.23
1	E	52	SER	N-CA-C	6.22	118.87	109.23
1	A	145	LYS	N-CA-C	-6.09	104.20	111.69
1	D	232	GLU	N-CA-C	-6.07	104.67	111.28
1	C	246	VAL	N-CA-C	-6.06	105.16	111.58
1	D	138	THR	N-CA-C	-6.00	104.95	112.93
1	C	197	MET	N-CA-C	5.95	122.39	114.12
1	D	247	GLU	N-CA-C	-5.92	104.75	111.14
1	C	233	THR	N-CA-C	-5.87	104.97	111.71
1	A	197	MET	N-CA-C	5.80	121.12	112.94
1	E	48	ARG	N-CA-C	-5.79	98.46	110.80
1	A	14	ASN	N-CA-C	-5.75	105.97	112.87
1	B	75	SER	N-CA-C	-5.74	104.02	111.02
1	A	49	GLU	N-CA-C	-5.73	98.59	110.80
1	F	81	LEU	N-CA-C	-5.72	103.86	111.24
1	D	8	HIS	N-CA-C	5.66	117.53	111.36
1	A	242	VAL	N-CA-C	-5.64	106.20	111.45
1	C	63	ILE	N-CA-C	5.64	117.94	108.81
1	B	99	GLN	CA-C-N	5.59	125.43	119.28
1	B	99	GLN	C-N-CA	5.59	125.43	119.28
1	B	92	ILE	N-CA-C	-5.58	99.77	108.86
1	F	194	ASN	N-CA-C	5.58	116.44	108.74
1	B	194	ASN	N-CA-C	5.57	116.42	108.74
1	C	215	MET	N-CA-C	5.55	117.15	107.49
1	A	243	LYS	N-CA-C	-5.51	104.30	111.02
1	C	17	GLN	N-CA-C	-5.50	104.15	111.02
1	D	48	ARG	CB-CA-C	-5.50	109.25	115.79
1	B	193	MET	N-CA-C	5.49	119.95	112.04
1	F	229	PRO	N-CA-C	5.49	119.31	111.13
1	B	248	ALA	N-CA-C	-5.48	106.43	113.23
1	E	76	ILE	N-CA-C	5.48	115.57	110.42
1	E	117	ASP	N-CA-C	-5.47	103.40	110.19
1	A	144	ALA	N-CA-C	-5.45	105.49	111.82
1	D	9	LEU	N-CA-C	5.45	119.99	113.23
1	A	83	GLN	N-CA-C	-5.43	105.52	111.82
1	B	199	SER	N-CA-C	5.42	117.95	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	228	ILE	CA-C-N	5.37	125.83	120.52
1	F	228	ILE	C-N-CA	5.37	125.83	120.52
1	B	189	ALA	N-CA-C	-5.35	105.34	111.07
1	B	49	GLU	N-CA-C	-5.31	105.64	113.61
1	E	9	LEU	N-CA-C	5.30	117.74	111.33
1	D	46	SER	N-CA-C	5.29	116.05	107.32
1	F	151	THR	N-CA-C	5.28	117.50	110.53
1	E	206	CYS	N-CA-C	-5.19	105.78	112.68
1	E	49	GLU	N-CA-C	-5.18	106.06	114.09
1	A	138	THR	N-CA-C	-5.18	105.71	112.23
1	C	151	THR	N-CA-C	5.17	117.67	109.24
1	E	146	SER	N-CA-C	5.17	119.86	113.50
1	C	222	ASN	N-CA-C	-5.14	98.90	107.99
1	D	122	HIS	N-CA-C	-5.10	106.75	113.17
1	A	111	THR	N-CA-C	-5.09	104.70	112.04
1	A	124	ALA	CA-C-N	5.09	126.21	119.84
1	A	124	ALA	C-N-CA	5.09	126.21	119.84
1	C	225	GLN	N-CA-C	-5.08	103.97	110.53
1	E	103	ASN	N-CA-C	5.08	117.98	110.46
1	F	154	GLY	N-CA-C	5.07	117.43	110.58
1	B	131	VAL	N-CA-C	5.07	116.26	108.71
1	A	167	GLU	N-CA-C	5.05	121.56	110.80
1	E	113	SER	N-CA-C	5.03	117.03	109.23

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	1877	0	1887	192	0
1	B	1877	0	1887	241	0
1	C	1877	0	1887	204	0
1	D	1877	0	1887	212	0
1	E	1877	0	1887	263	0
1	F	1877	0	1887	252	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	6	5	0
All	All	11270	0	11328	1300	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 58.

All (1300) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:HG2	1:B:236:GLN:HB2	1.27	1.16
1:E:167:GLU:HG3	1:E:183:SER:H	1.15	1.10
1:C:201:THR:HG22	1:C:205:MET:HE2	1.34	1.08
1:C:228:ILE:HB	1:C:229:PRO:HD2	1.37	1.06
1:C:104:VAL:HG11	1:C:229:PRO:HB3	1.34	1.06
1:E:22:ALA:HB2	1:E:86:ILE:HD13	1.36	1.05
1:C:222:ASN:HB3	1:C:225:GLN:HE21	1.21	1.05
1:C:16:LEU:HB3	1:C:19:ALA:HB3	1.40	1.03
1:C:21:LEU:HD23	1:C:22:ALA:H	1.19	1.01
1:B:21:LEU:HD23	1:B:22:ALA:N	1.75	1.01
1:F:54:ARG:HH11	1:F:54:ARG:HB3	1.23	0.99
1:D:171:THR:HG22	1:D:172:TYR:H	1.21	0.99
1:F:30:ARG:CZ	1:F:238:GLU:HG2	1.92	0.99
1:F:194:ASN:N	1:F:194:ASN:HD22	1.61	0.98
1:B:60:LYS:HD2	1:B:253:LEU:HB3	1.46	0.97
1:E:194:ASN:HD22	1:E:194:ASN:H	1.06	0.96
1:E:17:GLN:HE21	1:E:17:GLN:HA	1.29	0.96
1:A:16:LEU:HB3	1:A:63:ILE:HD11	1.45	0.95
1:B:33:LYS:HA	1:B:33:LYS:HE2	1.46	0.95
1:B:21:LEU:HD23	1:B:22:ALA:H	1.31	0.95
1:C:67:THR:HG21	1:C:91:ARG:HH12	1.31	0.95
1:D:16:LEU:HB3	1:D:63:ILE:HD11	1.49	0.93
1:D:21:LEU:HD12	1:D:88:THR:HB	1.50	0.93
1:D:147:ILE:HD11	1:D:149:ALA:HB2	1.51	0.93
1:E:242:VAL:O	1:E:246:VAL:HG23	1.69	0.92
1:E:31:VAL:HG13	1:E:64:VAL:HG12	1.52	0.92
1:C:54:ARG:HH11	1:C:54:ARG:HB3	1.33	0.91
1:F:57:LEU:HD11	1:F:250:ARG:NH1	1.85	0.90
1:E:90:LEU:HD11	1:E:252:LEU:HD12	1.54	0.90
1:B:94:THR:HG22	1:B:220:ILE:HG21	1.52	0.90
1:D:194:ASN:H	1:D:194:ASN:HD22	1.18	0.90
1:B:190:MET:HE1	1:F:125:PRO:HD3	1.50	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:HIS:O	1:E:244:ILE:HG12	1.72	0.89
1:E:17:GLN:HG3	1:E:54:ARG:HH21	1.35	0.89
1:F:38:MET:HB2	1:F:55:ALA:HB1	1.53	0.89
1:B:16:LEU:HD12	1:B:63:ILE:HG13	1.54	0.89
1:F:143:ALA:N	1:F:251:ARG:HH12	1.70	0.88
1:A:17:GLN:HG2	1:A:54:ARG:HE	1.36	0.88
1:C:21:LEU:HD23	1:C:22:ALA:N	1.86	0.88
1:E:11:LEU:HD22	1:E:44:LEU:HD22	1.55	0.88
1:E:87:ARG:HH11	1:E:87:ARG:HG3	1.39	0.88
1:B:9:LEU:HD11	1:B:81:LEU:HD23	1.55	0.87
1:A:242:VAL:O	1:A:246:VAL:HG23	1.74	0.87
1:A:117:ASP:HA	1:A:160:ASP:OD1	1.75	0.87
1:B:194:ASN:HD22	1:B:194:ASN:H	1.24	0.86
1:F:163:TYR:HA	1:F:168:ARG:HD2	1.57	0.85
2:B:254:ACY:H2	1:D:48:ARG:HH12	1.41	0.85
1:E:44:LEU:HD12	1:E:54:ARG:HB2	1.57	0.84
1:A:186:GLU:O	1:A:190:MET:HG3	1.76	0.84
1:D:30:ARG:O	1:D:34:ILE:HG12	1.77	0.84
1:A:105:GLY:HA2	1:A:237:THR:HG23	1.58	0.84
1:C:107:VAL:HG21	1:C:244:ILE:HD12	1.58	0.84
1:B:163:TYR:HA	1:B:168:ARG:HD2	1.59	0.84
1:D:31:VAL:HG13	1:D:64:VAL:HG12	1.58	0.84
1:A:196:GLU:CD	1:A:199:SER:H	1.86	0.84
1:D:76:ILE:HG22	1:D:80:GLU:HG3	1.59	0.84
1:B:158:SER:HB3	1:B:200:ALA:HB2	1.58	0.83
1:C:67:THR:HG21	1:C:91:ARG:NH1	1.93	0.83
1:A:108:LEU:HD13	1:A:193:MET:HG3	1.59	0.83
1:D:133:ASP:CG	1:D:212:ARG:HG2	2.03	0.83
1:A:179:ARG:HD2	1:A:180:PHE:CE1	2.12	0.83
1:F:194:ASN:HD22	1:F:194:ASN:H	1.23	0.83
1:A:156:THR:HG22	1:A:157:ALA:H	1.41	0.83
1:F:187:TRP:HB3	1:F:192:VAL:HG21	1.61	0.83
1:F:249:ALA:O	1:F:253:LEU:HG	1.79	0.82
1:A:6:VAL:HB	1:A:80:GLU:OE2	1.79	0.82
1:D:171:THR:HG22	1:D:172:TYR:N	1.96	0.81
1:F:240:HIS:O	1:F:244:ILE:HG12	1.80	0.81
1:B:25:PRO:HD2	1:B:65:CYS:O	1.79	0.81
1:E:15:ASP:O	1:E:44:LEU:HD11	1.81	0.81
1:E:57:LEU:HD21	1:E:250:ARG:HG2	1.62	0.81
1:F:44:LEU:HD11	1:F:54:ARG:HB2	1.60	0.81
1:A:91:ARG:O	1:A:91:ARG:HG3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ASN:HD22	1:B:194:ASN:N	1.78	0.80
1:F:30:ARG:NH2	1:F:238:GLU:HG2	1.96	0.80
1:E:194:ASN:HD22	1:E:194:ASN:N	1.79	0.80
1:B:126:MET:HE1	1:F:127:GLU:HG3	1.64	0.80
1:D:179:ARG:HH11	1:D:179:ARG:HB2	1.45	0.79
1:F:89:PHE:O	1:F:90:LEU:HG	1.82	0.79
1:E:169:TYR:OH	1:E:181:LYS:HG3	1.82	0.79
1:A:16:LEU:HB3	1:A:63:ILE:CD1	2.13	0.79
1:B:69:ILE:HD12	1:B:69:ILE:H	1.46	0.79
1:C:38:MET:HG3	1:C:57:LEU:HD13	1.63	0.79
1:C:231:ALA:O	1:C:234:MET:HB2	1.83	0.79
1:D:177:VAL:HG22	1:D:179:ARG:H	1.48	0.79
1:F:21:LEU:HD13	1:F:253:LEU:HD23	1.65	0.79
1:B:17:GLN:HG2	1:B:54:ARG:NH1	1.98	0.78
1:C:96:GLY:O	1:C:194:ASN:HB2	1.83	0.78
1:C:117:ASP:HA	1:C:160:ASP:HB2	1.64	0.78
1:C:44:LEU:HD11	1:C:54:ARG:HB2	1.64	0.78
1:F:54:ARG:HH11	1:F:54:ARG:CB	1.96	0.78
1:E:194:ASN:H	1:E:194:ASN:ND2	1.81	0.77
1:E:161:THR:OG1	1:E:165:GLY:HA3	1.84	0.77
1:F:114:VAL:HG11	1:F:187:TRP:CZ3	2.19	0.77
1:C:222:ASN:HB3	1:C:225:GLN:NE2	1.98	0.77
1:D:34:ILE:HD12	1:D:242:VAL:HG13	1.67	0.77
1:B:5:ASP:HB2	1:B:12:THR:HA	1.65	0.77
1:C:58:ASP:O	1:C:60:LYS:HG2	1.85	0.77
1:C:16:LEU:HD22	1:C:63:ILE:CD1	2.15	0.77
1:C:91:ARG:HB3	1:C:215:MET:HG3	1.67	0.77
1:F:236:GLN:HA	1:F:239:SER:OG	1.85	0.77
1:E:156:THR:HG23	1:E:194:ASN:ND2	1.99	0.76
1:D:161:THR:OG1	1:D:164:PRO:HG2	1.86	0.76
1:C:49:GLU:OE1	1:E:48:ARG:O	2.04	0.76
1:D:17:GLN:HE21	1:D:17:GLN:HA	1.50	0.76
1:D:247:GLU:O	1:D:250:ARG:HB2	1.86	0.76
1:B:137:THR:O	1:B:141:VAL:HG23	1.85	0.76
1:F:8:HIS:HB2	1:F:80:GLU:OE2	1.86	0.76
1:C:4:SER:N	1:C:12:THR:HG22	2.01	0.75
1:E:8:HIS:HB3	1:E:50:PHE:CE1	2.21	0.75
1:C:222:ASN:O	1:C:225:GLN:HB3	1.85	0.75
1:F:138:THR:O	1:F:142:GLU:HG3	1.86	0.75
1:B:26:GLY:HA3	2:B:254:ACY:H1	1.69	0.74
1:E:138:THR:O	1:E:142:GLU:HG3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:LEU:HD21	1:C:90:LEU:HD12	1.69	0.74
1:F:142:GLU:HB2	1:F:251:ARG:NH1	2.03	0.74
1:A:156:THR:HG22	1:A:157:ALA:N	2.03	0.74
1:C:144:ALA:O	1:C:147:ILE:HD13	1.88	0.74
1:D:89:PHE:O	1:D:213:ALA:HA	1.87	0.74
1:B:230:ASN:HB2	1:B:233:THR:OG1	1.89	0.73
1:D:22:ALA:HA	1:D:63:ILE:O	1.87	0.73
1:F:6:VAL:HG21	1:F:9:LEU:HB2	1.70	0.73
1:D:34:ILE:HD12	1:D:242:VAL:CG1	2.18	0.73
1:E:186:GLU:HG3	1:E:190:MET:HE1	1.71	0.72
1:E:22:ALA:CB	1:E:86:ILE:HD13	2.17	0.72
1:E:76:ILE:HA	1:E:79:GLU:OE1	1.88	0.72
1:E:86:ILE:O	1:E:87:ARG:HG3	1.88	0.72
1:A:48:ARG:HH11	1:A:48:ARG:HB3	1.52	0.72
1:F:229:PRO:HG2	1:F:234:MET:SD	2.29	0.72
1:E:115:ARG:NH1	1:E:126:MET:HA	2.04	0.72
1:F:22:ALA:HB2	1:F:86:ILE:HD12	1.69	0.72
1:F:220:ILE:O	1:F:229:PRO:HG3	1.88	0.72
1:F:104:VAL:HG21	1:F:227:GLU:OE1	1.90	0.72
1:C:54:ARG:HH11	1:C:54:ARG:CB	2.03	0.72
1:E:57:LEU:HD23	1:E:253:LEU:HD11	1.71	0.72
1:E:91:ARG:HG3	1:E:92:ILE:N	2.02	0.72
1:B:158:SER:CB	1:B:200:ALA:HB2	2.20	0.72
1:F:163:TYR:HA	1:F:168:ARG:CD	2.20	0.72
1:F:11:LEU:HD21	1:F:52:SER:OG	1.90	0.71
1:E:17:GLN:HG2	1:E:54:ARG:HE	1.54	0.71
1:B:149:ALA:CB	1:B:244:ILE:HD11	2.21	0.71
1:A:17:GLN:HG3	1:A:54:ARG:HH21	1.56	0.71
1:C:28:PRO:HG3	1:C:49:GLU:OE2	1.90	0.71
1:F:147:ILE:HD11	1:F:244:ILE:HD11	1.70	0.71
1:C:104:VAL:CG1	1:C:229:PRO:HB3	2.15	0.71
1:E:196:GLU:CD	1:E:199:SER:H	1.99	0.71
1:F:230:ASN:ND2	1:F:232:GLU:H	1.87	0.71
1:E:184:MET:O	1:E:188:GLN:HG3	1.91	0.71
1:B:71:GLY:N	1:B:72:PRO:HD3	2.06	0.71
1:D:175:ARG:NH1	1:D:177:VAL:HA	2.06	0.71
1:F:112:ALA:HB2	1:F:131:VAL:HA	1.70	0.71
1:B:126:MET:CE	1:F:127:GLU:HG3	2.21	0.71
1:C:107:VAL:HG21	1:C:244:ILE:CD1	2.19	0.70
1:F:99:GLN:HB2	1:F:102:ILE:HG12	1.73	0.70
1:A:43:LYS:HB2	1:A:53:TRP:CZ2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:GLU:OE1	1:F:238:GLU:N	2.24	0.70
1:D:96:GLY:HA2	1:D:221:VAL:O	1.90	0.70
1:A:12:THR:O	1:A:84:LEU:HD22	1.91	0.70
1:A:67:THR:HG21	1:A:74:THR:HG23	1.74	0.70
1:B:94:THR:HG22	1:B:220:ILE:HD13	1.73	0.70
1:F:196:GLU:OE2	1:F:198:GLU:N	2.24	0.70
1:B:151:THR:O	1:B:152:HIS:HD2	1.75	0.70
1:F:140:LEU:HD13	1:F:216:VAL:HB	1.74	0.70
1:C:25:PRO:HD2	1:C:65:CYS:O	1.92	0.70
1:E:93:GLY:O	1:E:217:ALA:HA	1.92	0.70
1:F:112:ALA:HA	1:F:130:ALA:O	1.92	0.69
1:B:164:PRO:C	1:B:166:GLN:H	2.00	0.69
1:C:54:ARG:HB3	1:C:54:ARG:NH1	2.07	0.69
1:D:171:THR:CG2	1:D:172:TYR:H	2.03	0.69
1:F:177:VAL:HG22	1:F:178:ARG:H	1.57	0.69
1:C:54:ARG:HG3	1:C:62:VAL:O	1.92	0.69
1:F:54:ARG:HB3	1:F:54:ARG:NH1	2.02	0.69
1:C:26:GLY:HA2	1:C:67:THR:OG1	1.92	0.69
1:D:72:PRO:O	1:D:75:SER:HB3	1.92	0.69
1:A:37:LEU:N	1:A:37:LEU:HD22	2.08	0.69
1:B:127:GLU:N	1:F:126:MET:HE1	2.08	0.69
1:E:8:HIS:HB3	1:E:50:PHE:CD1	2.28	0.69
1:D:63:ILE:HD12	1:D:86:ILE:HD11	1.74	0.68
1:D:98:ILE:HG12	1:D:193:MET:O	1.93	0.68
1:E:21:LEU:HD23	1:E:22:ALA:N	2.07	0.68
1:E:27:ASP:OD2	1:E:29:GLU:HB2	1.93	0.68
1:E:38:MET:O	1:F:145:LYS:HE3	1.93	0.68
1:B:17:GLN:HA	1:B:17:GLN:HE21	1.58	0.68
1:C:79:GLU:O	1:C:83:GLN:HG3	1.92	0.68
1:D:136:CYS:SG	1:D:212:ARG:HB3	2.34	0.68
1:F:196:GLU:CD	1:F:199:SER:H	2.00	0.68
1:A:137:THR:O	1:A:141:VAL:HG23	1.94	0.68
1:D:87:ARG:HH21	1:D:212:ARG:HH22	1.40	0.68
1:F:108:LEU:HD13	1:F:193:MET:HB3	1.76	0.68
1:C:49:GLU:OE2	1:C:49:GLU:HA	1.93	0.68
1:D:228:ILE:N	1:D:228:ILE:HD13	2.08	0.68
1:B:232:GLU:HG3	1:B:235:LYS:HD3	1.76	0.68
1:B:35:ALA:HA	1:B:38:MET:HE3	1.76	0.67
1:B:104:VAL:HA	1:B:219:VAL:HG12	1.76	0.67
1:E:15:ASP:HB3	1:E:44:LEU:HD21	1.75	0.67
1:D:111:THR:O	1:D:131:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:GLN:HG3	1:E:54:ARG:NH2	2.10	0.67
1:E:94:THR:O	1:E:95:THR:HB	1.94	0.67
1:A:251:ARG:H	1:A:251:ARG:HD2	1.59	0.67
1:B:212:ARG:NH2	1:B:252:LEU:HD22	2.08	0.67
1:A:159:SER:OG	1:A:165:GLY:HA3	1.94	0.67
1:E:161:THR:CB	1:E:165:GLY:HA3	2.25	0.67
1:C:175:ARG:NH2	1:E:208:SER:HB2	2.09	0.67
1:D:112:ALA:O	1:D:155:VAL:HG13	1.95	0.67
1:E:76:ILE:O	1:E:79:GLU:HG2	1.94	0.67
1:C:98:ILE:HG12	1:C:193:MET:O	1.95	0.67
1:C:228:ILE:HB	1:C:229:PRO:CD	2.21	0.67
1:D:194:ASN:HD22	1:D:194:ASN:N	1.89	0.67
1:F:126:MET:O	1:F:126:MET:SD	2.54	0.67
1:F:194:ASN:N	1:F:194:ASN:ND2	2.34	0.67
1:A:17:GLN:HG2	1:A:54:ARG:NE	2.09	0.66
1:E:159:SER:O	1:E:197:MET:HG2	1.95	0.66
1:F:25:PRO:O	1:F:66:SER:HA	1.95	0.66
1:A:11:LEU:HD21	1:A:52:SER:OG	1.96	0.66
1:E:44:LEU:H	1:E:53:TRP:HA	1.61	0.66
1:F:57:LEU:HD11	1:F:250:ARG:HH11	1.59	0.66
1:A:15:ASP:HB3	1:A:16:LEU:HD23	1.76	0.66
1:F:229:PRO:O	1:F:234:MET:HE1	1.94	0.66
1:B:124:ALA:HA	1:D:175:ARG:HE	1.61	0.66
1:E:186:GLU:HG3	1:E:190:MET:CE	2.25	0.66
1:D:12:THR:HB	1:D:15:ASP:OD2	1.96	0.65
1:E:167:GLU:CG	1:E:183:SER:H	2.01	0.65
1:C:242:VAL:O	1:C:246:VAL:HG23	1.96	0.65
1:F:6:VAL:HB	1:F:80:GLU:OE1	1.95	0.65
1:B:159:SER:HB3	1:B:166:GLN:HE21	1.61	0.65
1:F:104:VAL:HG22	1:F:222:ASN:HB2	1.77	0.65
1:B:144:ALA:O	1:B:149:ALA:HB3	1.96	0.65
1:B:194:ASN:N	1:B:194:ASN:ND2	2.44	0.65
1:D:178:ARG:NH2	1:D:181:LYS:NZ	2.44	0.65
1:F:145:LYS:C	1:F:147:ILE:H	2.05	0.65
1:D:87:ARG:HH21	1:D:212:ARG:NH2	1.95	0.65
1:B:115:ARG:NH2	1:B:121:LEU:HD23	2.12	0.65
1:B:164:PRO:HG2	1:B:165:GLY:H	1.61	0.65
1:E:69:ILE:HD13	1:E:69:ILE:N	2.11	0.65
1:E:239:SER:HA	1:E:242:VAL:HG23	1.78	0.65
1:A:162:PHE:HB2	1:A:197:MET:SD	2.37	0.65
1:B:69:ILE:HD12	1:B:69:ILE:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ILE:HD11	1:B:192:VAL:O	1.97	0.65
1:D:104:VAL:O	1:D:233:THR:HG21	1.96	0.65
1:B:15:ASP:O	1:B:54:ARG:HD3	1.96	0.64
1:B:89:PHE:C	1:B:90:LEU:HD12	2.22	0.64
1:F:38:MET:CB	1:F:55:ALA:HB1	2.27	0.64
1:F:184:MET:O	1:F:188:GLN:HB2	1.97	0.64
1:B:89:PHE:O	1:B:90:LEU:HD12	1.97	0.64
1:D:151:THR:HG22	1:D:152:HIS:N	2.11	0.64
1:D:67:THR:HG22	1:D:77:ALA:CB	2.27	0.64
1:A:86:ILE:O	1:A:87:ARG:HG2	1.98	0.64
1:C:13:LYS:HE3	1:C:84:LEU:O	1.97	0.64
1:A:136:CYS:O	1:A:140:LEU:HG	1.97	0.64
1:D:91:ARG:HB3	1:D:215:MET:HG2	1.80	0.64
1:E:184:MET:HE3	1:E:188:GLN:NE2	2.13	0.64
1:F:196:GLU:OE2	1:F:199:SER:N	2.26	0.64
1:B:71:GLY:N	1:B:72:PRO:CD	2.61	0.64
1:B:168:ARG:CZ	1:B:223:ARG:HH22	2.11	0.64
1:C:21:LEU:HD21	1:C:90:LEU:CD1	2.28	0.63
1:D:163:TYR:N	1:D:164:PRO:HD2	2.13	0.63
1:E:237:THR:HA	1:E:240:HIS:CD2	2.33	0.63
1:F:132:ALA:HB2	1:F:203:LEU:HD22	1.80	0.63
1:F:161:THR:HB	1:F:164:PRO:HG2	1.79	0.63
1:F:162:PHE:O	1:F:168:ARG:HD2	1.98	0.63
1:A:117:ASP:CA	1:A:160:ASP:OD1	2.45	0.63
1:E:57:LEU:HD11	1:E:250:ARG:HG2	1.81	0.63
1:D:40:LYS:O	1:D:42:VAL:HG23	1.98	0.63
1:D:87:ARG:HA	1:D:211:LEU:HD22	1.80	0.63
1:F:34:ILE:HD13	1:F:242:VAL:HG13	1.80	0.63
1:F:163:TYR:CG	1:F:168:ARG:HD3	2.33	0.63
1:B:62:VAL:HG22	1:B:253:LEU:HD11	1.81	0.63
1:B:108:LEU:HB3	1:B:193:MET:CE	2.29	0.63
1:B:169:TYR:O	1:B:171:THR:N	2.29	0.63
1:E:76:ILE:O	1:E:80:GLU:HG2	1.99	0.63
1:F:144:ALA:HA	1:F:244:ILE:HD12	1.80	0.63
1:A:177:VAL:O	1:A:181:LYS:HG3	1.99	0.63
1:B:94:THR:CG2	1:B:220:ILE:HD13	2.28	0.63
1:C:158:SER:HB3	1:C:200:ALA:HB2	1.79	0.63
1:D:175:ARG:CZ	1:D:177:VAL:HA	2.28	0.63
1:A:131:VAL:HG22	1:A:132:ALA:N	2.14	0.62
1:A:201:THR:O	1:A:205:MET:HB3	1.99	0.62
1:A:241:ALA:HA	1:A:244:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLU:CD	1:B:59:GLY:HA2	2.24	0.62
1:B:138:THR:O	1:B:142:GLU:HG3	1.98	0.62
1:E:147:ILE:C	1:E:147:ILE:HD13	2.24	0.62
1:B:186:GLU:CD	1:B:190:MET:HE3	2.24	0.62
1:B:108:LEU:HB3	1:B:193:MET:HE2	1.80	0.62
1:C:132:ALA:HA	1:C:203:LEU:HD22	1.82	0.62
1:F:176:VAL:HG12	1:F:177:VAL:H	1.65	0.62
1:E:196:GLU:O	1:E:197:MET:HG3	1.97	0.62
1:A:101:HIS:CE1	1:A:102:ILE:HG13	2.34	0.62
1:B:235:LYS:HA	1:B:238:GLU:OE1	2.00	0.62
1:F:142:GLU:O	1:F:145:LYS:HB3	1.99	0.62
1:E:22:ALA:HB2	1:E:86:ILE:CD1	2.21	0.62
1:E:49:GLU:HA	1:E:49:GLU:OE2	1.99	0.62
1:E:247:GLU:OE2	1:E:250:ARG:NE	2.33	0.62
1:F:34:ILE:O	1:F:36:ALA:N	2.33	0.62
1:C:25:PRO:O	1:C:67:THR:HG23	2.00	0.61
1:E:17:GLN:CG	1:E:54:ARG:HE	2.13	0.61
1:A:48:ARG:HB3	1:A:48:ARG:NH1	2.15	0.61
1:C:38:MET:HB3	1:C:56:GLU:O	2.00	0.61
1:E:63:ILE:HD12	1:E:86:ILE:HD11	1.82	0.61
1:F:29:GLU:O	1:F:30:ARG:C	2.43	0.61
1:E:175:ARG:HD2	1:E:176:VAL:N	2.15	0.61
1:E:42:VAL:O	1:E:43:LYS:C	2.43	0.61
1:F:120:SER:HB3	1:F:201:THR:HA	1.82	0.61
1:A:196:GLU:CD	1:A:198:GLU:H	2.08	0.61
1:B:126:MET:HE1	1:F:127:GLU:HA	1.83	0.61
1:E:63:ILE:HG22	1:E:64:VAL:N	2.14	0.61
1:B:104:VAL:HA	1:B:219:VAL:CG1	2.31	0.61
1:C:143:ALA:O	1:C:147:ILE:HG23	2.01	0.61
1:F:78:VAL:HG11	1:F:205:MET:SD	2.41	0.61
1:A:21:LEU:HD23	1:A:22:ALA:N	2.16	0.61
1:C:79:GLU:HG3	1:C:83:GLN:HE21	1.64	0.60
1:C:233:THR:HA	1:C:236:GLN:HG3	1.81	0.60
1:E:167:GLU:HG3	1:E:183:SER:N	2.00	0.60
1:A:28:PRO:HB3	1:A:49:GLU:O	2.01	0.60
1:E:141:VAL:O	1:E:145:LYS:HB2	2.01	0.60
1:B:88:THR:HA	1:B:212:ARG:HB2	1.84	0.60
1:C:27:ASP:HA	1:E:48:ARG:NH1	2.15	0.60
1:B:23:ILE:HG22	1:B:24:VAL:N	2.15	0.60
1:A:226:GLN:NE2	1:A:227:GLU:H	1.99	0.60
1:C:220:ILE:HG13	1:C:234:MET:SD	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:MET:HA	1:F:195:TYR:OH	2.02	0.60
1:B:8:HIS:HB3	1:B:50:PHE:CE1	2.36	0.60
1:C:123:PHE:HA	1:E:175:ARG:HH21	1.65	0.60
1:A:13:LYS:C	1:A:15:ASP:H	2.10	0.60
1:A:116:LEU:HB2	1:A:158:SER:O	2.01	0.60
1:E:139:ALA:CB	1:E:252:LEU:HD21	2.31	0.60
1:F:163:TYR:CD2	1:F:168:ARG:HD3	2.37	0.60
1:A:247:GLU:O	1:A:250:ARG:HB2	2.01	0.60
1:C:137:THR:O	1:C:141:VAL:HG23	2.01	0.60
1:D:87:ARG:NH2	1:D:212:ARG:HH22	2.00	0.60
1:D:90:LEU:HD21	1:D:252:LEU:CD1	2.32	0.60
1:E:96:GLY:HA2	1:E:221:VAL:O	2.02	0.60
1:F:247:GLU:OE2	1:F:250:ARG:NE	2.33	0.60
1:A:132:ALA:HA	1:A:203:LEU:HD22	1.83	0.60
1:B:102:ILE:HG12	1:B:152:HIS:CE1	2.37	0.60
1:B:102:ILE:HG12	1:B:152:HIS:ND1	2.17	0.60
1:F:62:VAL:HG12	1:F:63:ILE:N	2.17	0.60
1:F:227:GLU:O	1:F:228:ILE:HG23	2.02	0.60
1:C:229:PRO:HB2	1:C:233:THR:HB	1.82	0.59
1:B:246:VAL:O	1:B:249:ALA:HB3	2.01	0.59
1:C:78:VAL:HG13	1:C:89:PHE:CZ	2.36	0.59
1:E:216:VAL:HG13	1:E:216:VAL:O	2.01	0.59
1:C:228:ILE:CB	1:C:229:PRO:HD2	2.23	0.59
1:E:92:ILE:HD12	1:E:93:GLY:H	1.66	0.59
1:A:23:ILE:O	1:A:64:VAL:HA	2.02	0.59
1:C:38:MET:HB2	1:C:55:ALA:HB1	1.85	0.59
1:D:147:ILE:C	1:D:147:ILE:HD12	2.28	0.59
1:E:25:PRO:O	1:E:66:SER:HA	2.02	0.59
1:E:136:CYS:O	1:E:140:LEU:HG	2.03	0.59
1:F:29:GLU:O	1:F:32:GLU:N	2.34	0.59
1:C:163:TYR:HD2	1:C:171:THR:HG22	1.67	0.59
1:D:171:THR:C	1:D:173:SER:H	2.10	0.59
1:C:30:ARG:HD3	1:C:33:LYS:HG3	1.82	0.59
1:C:172:TYR:HB2	1:E:83:GLN:HG3	1.85	0.59
1:C:237:THR:C	1:C:239:SER:H	2.11	0.59
1:D:162:PHE:HA	1:D:166:GLN:HE21	1.66	0.59
1:E:23:ILE:HD13	1:E:90:LEU:HB2	1.83	0.59
1:F:92:ILE:HD11	1:F:241:ALA:HB1	1.84	0.59
1:B:21:LEU:CD2	1:B:22:ALA:N	2.61	0.59
1:D:95:THR:O	1:D:219:VAL:HA	2.03	0.59
1:C:26:GLY:C	1:E:48:ARG:HH12	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ILE:HG22	1:B:24:VAL:H	1.68	0.58
1:B:60:LYS:CD	1:B:253:LEU:HB3	2.27	0.58
1:A:18:GLY:O	1:A:19:ALA:C	2.45	0.58
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.68	0.58
1:B:24:VAL:HG23	1:B:24:VAL:O	2.03	0.58
1:D:6:VAL:HB	1:D:80:GLU:OE1	2.02	0.58
1:A:87:ARG:HA	1:A:211:LEU:HD22	1.85	0.58
1:B:105:GLY:HA2	1:B:237:THR:HG23	1.85	0.58
1:B:122:HIS:O	1:D:175:ARG:O	2.22	0.58
1:C:9:LEU:HD11	1:C:81:LEU:HG	1.86	0.58
1:C:162:PHE:HA	1:C:166:GLN:NE2	2.19	0.58
1:D:79:GLU:O	1:D:83:GLN:HB2	2.03	0.58
1:E:39:ASP:O	1:E:40:LYS:HB2	2.03	0.58
1:F:221:VAL:HG22	1:F:223:ARG:N	2.18	0.58
1:B:24:VAL:HA	1:B:65:CYS:O	2.04	0.58
1:E:90:LEU:HD11	1:E:252:LEU:CD1	2.31	0.58
1:C:67:THR:CG2	1:C:91:ARG:HH12	2.13	0.58
1:C:136:CYS:HA	1:C:252:LEU:HD11	1.85	0.58
1:E:11:LEU:CD2	1:E:44:LEU:HD22	2.28	0.58
1:B:35:ALA:HA	1:B:38:MET:CE	2.33	0.58
1:C:94:THR:CG2	1:C:220:ILE:HB	2.34	0.58
1:C:160:ASP:O	1:E:72:PRO:HB3	2.03	0.58
1:E:24:VAL:HA	1:E:65:CYS:O	2.04	0.58
1:A:151:THR:HG22	1:A:152:HIS:N	2.19	0.58
1:A:245:VAL:HA	1:A:248:ALA:HB3	1.86	0.58
1:B:186:GLU:HG2	1:B:190:MET:HE3	1.86	0.58
1:E:40:LYS:N	1:E:41:PRO:CD	2.65	0.58
1:A:72:PRO:O	1:A:76:ILE:HG12	2.04	0.58
1:E:46:SER:HA	1:E:51:THR:HA	1.85	0.58
1:F:183:SER:O	1:F:186:GLU:HB3	2.02	0.58
1:A:155:VAL:HG23	1:A:192:VAL:HA	1.85	0.58
1:B:31:VAL:HG12	1:B:53:TRP:HB2	1.86	0.58
1:E:216:VAL:HG11	1:E:245:VAL:HB	1.86	0.58
1:F:94:THR:O	1:F:95:THR:HB	2.03	0.58
1:A:95:THR:OG1	1:A:96:GLY:N	2.36	0.57
1:A:221:VAL:HG13	1:A:221:VAL:O	2.02	0.57
1:C:201:THR:O	1:C:205:MET:HG2	2.04	0.57
1:E:158:SER:HB3	1:E:200:ALA:HB2	1.84	0.57
1:B:23:ILE:O	1:B:24:VAL:HG13	2.04	0.57
1:B:228:ILE:HD13	1:B:228:ILE:H	1.69	0.57
1:C:21:LEU:CD2	1:C:22:ALA:N	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ILE:O	1:C:224:THR:HG21	2.04	0.57
1:F:6:VAL:CG2	1:F:9:LEU:HB2	2.34	0.57
1:A:225:GLN:HG2	1:A:226:GLN:N	2.19	0.57
1:A:239:SER:O	1:A:242:VAL:HB	2.05	0.57
1:B:15:ASP:HB3	1:B:44:LEU:HD22	1.86	0.57
1:E:177:VAL:CG1	1:E:180:PHE:HB2	2.33	0.57
1:F:247:GLU:CD	1:F:250:ARG:HH21	2.12	0.57
1:A:180:PHE:HA	1:A:183:SER:HB2	1.85	0.57
1:A:240:HIS:O	1:A:244:ILE:HG13	2.04	0.57
1:D:99:GLN:HA	1:D:99:GLN:OE1	2.05	0.57
1:A:17:GLN:CG	1:A:54:ARG:HE	2.11	0.57
1:B:169:TYR:HE2	1:B:176:VAL:HG23	1.70	0.57
1:D:16:LEU:CB	1:D:63:ILE:HD11	2.29	0.57
1:F:220:ILE:HG13	1:F:221:VAL:N	2.19	0.57
1:B:242:VAL:O	1:B:245:VAL:HG12	2.05	0.57
1:E:232:GLU:HG3	1:E:236:GLN:OE1	2.04	0.57
1:C:38:MET:HG3	1:C:57:LEU:HB2	1.85	0.57
1:B:17:GLN:HA	1:B:17:GLN:NE2	2.19	0.57
1:C:147:ILE:HD12	1:C:244:ILE:HG12	1.85	0.57
1:E:87:ARG:HG3	1:E:87:ARG:NH1	2.15	0.57
1:E:199:SER:HB3	1:E:215:MET:HE2	1.85	0.57
1:B:43:LYS:HB2	1:B:53:TRP:CZ2	2.40	0.57
1:E:137:THR:O	1:E:141:VAL:HG23	2.04	0.57
1:D:170:ASP:O	1:D:171:THR:OG1	2.22	0.57
1:F:97:ALA:CB	1:F:102:ILE:HB	2.35	0.57
1:C:169:TYR:C	1:C:171:THR:H	2.12	0.56
1:F:21:LEU:HG	1:F:88:THR:HB	1.86	0.56
1:B:90:LEU:HD23	1:B:140:LEU:HD21	1.87	0.56
1:B:91:ARG:HB3	1:B:215:MET:HG3	1.86	0.56
1:C:62:VAL:CG1	1:C:63:ILE:N	2.67	0.56
1:C:156:THR:HG23	1:C:194:ASN:O	2.05	0.56
1:D:16:LEU:HD22	1:D:63:ILE:CD1	2.35	0.56
1:D:159:SER:HB2	1:D:195:TYR:HE1	1.70	0.56
1:A:244:ILE:O	1:A:248:ALA:N	2.28	0.56
1:C:229:PRO:O	1:C:230:ASN:HB2	2.04	0.56
1:D:228:ILE:HD13	1:D:228:ILE:H	1.70	0.56
1:E:176:VAL:HG12	1:E:180:PHE:HB3	1.85	0.56
1:F:5:ASP:HB2	1:F:12:THR:HA	1.85	0.56
1:F:233:THR:C	1:F:235:LYS:H	2.11	0.56
1:B:128:PHE:CD1	1:B:129:PRO:HD2	2.40	0.56
1:C:126:MET:O	1:C:126:MET:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:ARG:HB3	1:F:170:ASP:OD2	2.05	0.56
1:B:144:ALA:CB	1:B:244:ILE:HD13	2.36	0.56
1:D:82:ALA:HB2	1:D:89:PHE:CZ	2.41	0.56
1:D:242:VAL:O	1:D:246:VAL:HG23	2.05	0.56
1:F:39:ASP:HB2	1:F:56:GLU:HB3	1.87	0.56
1:F:106:ASP:OD1	1:F:106:ASP:N	2.38	0.56
1:F:114:VAL:HG12	1:F:116:LEU:HG	1.88	0.56
1:A:23:ILE:HB	1:A:64:VAL:HG12	1.87	0.56
1:A:156:THR:HG23	1:A:194:ASN:CG	2.30	0.56
1:D:232:GLU:HG3	1:D:236:GLN:OE1	2.05	0.56
1:F:56:GLU:HA	1:F:60:LYS:O	2.04	0.56
1:A:17:GLN:CG	1:A:54:ARG:HH21	2.18	0.56
1:B:47:HIS:O	1:B:48:ARG:C	2.48	0.56
1:A:151:THR:HG22	1:A:152:HIS:H	1.71	0.56
1:B:12:THR:O	1:B:14:ASN:N	2.33	0.56
1:B:104:VAL:HG13	1:B:219:VAL:O	2.06	0.56
1:A:196:GLU:OE2	1:A:199:SER:N	2.35	0.56
1:C:149:ALA:O	1:C:151:THR:N	2.39	0.56
1:B:13:LYS:HE2	1:B:84:LEU:O	2.06	0.55
1:B:48:ARG:HH22	1:D:26:GLY:C	2.14	0.55
1:B:49:GLU:OE2	1:B:49:GLU:HA	2.06	0.55
1:B:114:VAL:HG22	1:F:128:PHE:HA	1.88	0.55
1:D:184:MET:HE3	1:D:188:GLN:OE1	2.05	0.55
1:D:158:SER:HB3	1:D:200:ALA:HB2	1.88	0.55
1:E:161:THR:HB	1:E:165:GLY:HA3	1.88	0.55
1:F:98:ILE:HD12	1:F:195:TYR:CD2	2.41	0.55
1:A:81:LEU:O	1:A:84:LEU:HB2	2.06	0.55
1:B:28:PRO:HG3	1:B:49:GLU:CD	2.32	0.55
1:B:228:ILE:HB	1:B:229:PRO:HD2	1.88	0.55
1:C:138:THR:O	1:C:142:GLU:HG3	2.07	0.55
1:D:156:THR:CB	1:D:194:ASN:HD21	2.19	0.55
1:D:187:TRP:HA	1:D:187:TRP:CE3	2.42	0.55
1:A:24:VAL:O	1:A:24:VAL:HG23	2.07	0.55
1:A:49:GLU:CG	1:F:49:GLU:HG2	2.37	0.55
1:A:113:SER:OG	1:A:156:THR:HB	2.06	0.55
1:A:227:GLU:O	1:A:228:ILE:C	2.50	0.55
1:B:142:GLU:CD	1:E:42:VAL:HG13	2.32	0.55
1:E:177:VAL:HG13	1:E:180:PHE:HB2	1.88	0.55
1:E:239:SER:HA	1:E:242:VAL:CG2	2.36	0.55
1:F:237:THR:HB	1:F:238:GLU:OE1	2.05	0.55
1:B:30:ARG:HH12	1:B:93:GLY:HA2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLU:HG2	1:B:53:TRP:CZ2	2.41	0.55
1:B:34:ILE:HD13	1:B:242:VAL:HG13	1.88	0.55
1:A:56:GLU:HG2	1:A:57:LEU:H	1.71	0.55
1:B:128:PHE:HA	1:F:114:VAL:HG22	1.88	0.55
1:F:63:ILE:CG2	1:F:64:VAL:N	2.69	0.55
1:A:35:ALA:HA	1:A:38:MET:HE3	1.87	0.55
1:A:178:ARG:HA	1:A:181:LYS:HE2	1.88	0.55
1:B:57:LEU:HG	1:B:250:ARG:HG2	1.89	0.55
1:B:102:ILE:HG12	1:B:152:HIS:HD1	1.72	0.55
1:B:166:GLN:HG2	1:B:195:TYR:CD1	2.42	0.55
1:C:177:VAL:O	1:C:178:ARG:C	2.50	0.55
1:D:166:GLN:NE2	1:D:168:ARG:HH22	2.04	0.55
1:E:7:PHE:O	1:E:9:LEU:N	2.40	0.55
1:B:196:GLU:CD	1:B:199:SER:H	2.15	0.55
1:D:242:VAL:O	1:D:245:VAL:HG12	2.07	0.55
1:E:44:LEU:HB2	1:E:53:TRP:O	2.07	0.55
1:F:62:VAL:CG1	1:F:63:ILE:N	2.70	0.55
1:B:23:ILE:O	1:B:24:VAL:CG1	2.55	0.55
1:D:109:VAL:O	1:D:193:MET:HE1	2.06	0.55
1:D:154:GLY:C	1:D:193:MET:HE2	2.31	0.55
1:A:160:ASP:HB3	1:F:119:ALA:HB2	1.89	0.55
1:F:196:GLU:OE2	1:F:197:MET:N	2.40	0.55
1:F:37:LEU:HD22	1:F:242:VAL:HG12	1.88	0.54
1:F:145:LYS:C	1:F:147:ILE:N	2.64	0.54
1:A:15:ASP:OD1	1:A:44:LEU:HD13	2.07	0.54
1:E:158:SER:HB2	1:E:199:SER:HG	1.71	0.54
1:C:87:ARG:HA	1:C:211:LEU:HD22	1.88	0.54
1:E:54:ARG:NH1	1:E:54:ARG:HG2	2.23	0.54
1:E:71:GLY:N	1:E:72:PRO:CD	2.70	0.54
1:B:177:VAL:O	1:B:178:ARG:C	2.51	0.54
1:D:31:VAL:HG13	1:D:64:VAL:CG1	2.35	0.54
1:E:139:ALA:HB2	1:E:252:LEU:HD21	1.89	0.54
1:A:143:ALA:O	1:A:146:SER:HB3	2.08	0.54
1:A:223:ARG:O	1:A:225:GLN:N	2.41	0.54
1:B:106:ASP:O	1:B:219:VAL:HG23	2.07	0.54
1:B:107:VAL:HG11	1:B:149:ALA:HB1	1.89	0.54
1:C:131:VAL:HG22	1:C:132:ALA:O	2.08	0.54
1:E:21:LEU:HD23	1:E:21:LEU:C	2.32	0.54
1:B:123:PHE:O	1:D:175:ARG:HD3	2.07	0.54
1:B:124:ALA:CA	1:D:175:ARG:HE	2.20	0.54
1:E:92:ILE:HG13	1:E:93:GLY:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ILE:HG12	1:E:193:MET:O	2.07	0.54
1:E:243:LYS:O	1:E:244:ILE:C	2.50	0.54
1:F:50:PHE:CD2	1:F:50:PHE:N	2.74	0.54
1:F:234:MET:O	1:F:238:GLU:OE2	2.25	0.54
1:A:167:GLU:O	1:A:167:GLU:HG2	2.07	0.54
1:B:9:LEU:HD13	1:B:11:LEU:HD12	1.87	0.54
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.73	0.54
1:D:231:ALA:HA	1:D:234:MET:HE2	1.89	0.54
1:E:15:ASP:C	1:E:16:LEU:HD23	2.33	0.54
1:F:158:SER:HA	1:F:196:GLU:O	2.08	0.54
1:A:176:VAL:O	1:A:181:LYS:HG2	2.08	0.54
1:B:162:PHE:O	1:B:168:ARG:NE	2.40	0.54
1:B:209:GLN:NE2	1:D:174:GLY:HA2	2.23	0.54
1:C:31:VAL:HG12	1:C:53:TRP:HB2	1.90	0.54
1:D:162:PHE:HA	1:D:166:GLN:NE2	2.23	0.54
1:E:24:VAL:HG23	1:E:24:VAL:O	2.07	0.54
1:E:87:ARG:HH11	1:E:87:ARG:CG	2.16	0.54
1:F:15:ASP:HB3	1:F:44:LEU:HD22	1.90	0.54
1:F:49:GLU:C	1:F:50:PHE:HD2	2.16	0.54
1:F:145:LYS:O	1:F:147:ILE:N	2.40	0.54
1:A:13:LYS:C	1:A:15:ASP:N	2.63	0.54
1:B:56:GLU:OE1	1:B:59:GLY:HA2	2.08	0.54
1:C:92:ILE:C	1:C:92:ILE:HD13	2.33	0.54
1:D:74:THR:O	1:D:78:VAL:HG23	2.07	0.54
1:F:34:ILE:O	1:F:37:LEU:N	2.40	0.54
1:F:157:ALA:O	1:F:195:TYR:HA	2.06	0.54
1:A:132:ALA:CA	1:A:203:LEU:HD22	2.38	0.54
1:D:82:ALA:HB2	1:D:89:PHE:HZ	1.73	0.54
1:E:91:ARG:NH2	1:E:198:GLU:OE1	2.41	0.54
1:F:63:ILE:HG22	1:F:64:VAL:N	2.23	0.54
1:F:132:ALA:HB2	1:F:203:LEU:CD2	2.38	0.54
1:C:38:MET:CB	1:C:55:ALA:HB1	2.38	0.53
1:C:49:GLU:HG2	1:E:49:GLU:OE2	2.07	0.53
1:D:16:LEU:HD11	1:D:84:LEU:HB3	1.90	0.53
1:D:156:THR:HG23	1:D:194:ASN:ND2	2.23	0.53
1:D:176:VAL:O	1:D:177:VAL:C	2.52	0.53
1:E:28:PRO:HA	1:E:31:VAL:HG23	1.89	0.53
1:A:28:PRO:HA	1:A:31:VAL:HG23	1.90	0.53
1:A:111:THR:O	1:A:131:VAL:HG23	2.08	0.53
1:A:222:ASN:HB3	1:A:225:GLN:HB3	1.89	0.53
1:D:89:PHE:HE1	1:D:211:LEU:HD13	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ASN:H	1:D:194:ASN:ND2	1.98	0.53
1:D:245:VAL:HG13	1:D:246:VAL:N	2.22	0.53
1:E:17:GLN:HA	1:E:17:GLN:NE2	2.11	0.53
1:F:92:ILE:HD11	1:F:241:ALA:CB	2.38	0.53
1:B:17:GLN:HE21	1:B:17:GLN:CA	2.20	0.53
1:E:88:THR:HA	1:E:212:ARG:O	2.09	0.53
1:F:82:ALA:HA	1:F:86:ILE:O	2.09	0.53
1:A:95:THR:HG22	1:A:217:ALA:HB1	1.90	0.53
1:B:115:ARG:HH21	1:B:121:LEU:HD23	1.74	0.53
1:C:39:ASP:O	1:C:40:LYS:C	2.52	0.53
1:D:178:ARG:NH2	1:D:181:LYS:HZ1	2.07	0.53
1:E:142:GLU:OE1	1:E:251:ARG:HD2	2.09	0.53
1:A:53:TRP:HB2	1:A:64:VAL:HG23	1.90	0.53
1:B:71:GLY:H	1:B:72:PRO:HD3	1.73	0.53
1:C:7:PHE:N	1:C:80:GLU:OE2	2.42	0.53
1:D:15:ASP:OD2	1:D:15:ASP:N	2.42	0.53
1:E:34:ILE:HG22	1:E:64:VAL:HG21	1.91	0.53
1:E:216:VAL:HG21	1:E:244:ILE:HG21	1.91	0.53
1:A:128:PHE:CD1	1:A:129:PRO:HD2	2.44	0.53
1:C:19:ALA:HA	1:C:61:ALA:O	2.08	0.53
1:D:89:PHE:CE1	1:D:211:LEU:HD13	2.42	0.53
1:A:196:GLU:OE2	1:A:198:GLU:N	2.41	0.53
1:B:111:THR:OG1	1:F:131:VAL:HG21	2.09	0.53
1:B:40:LYS:HD2	1:B:56:GLU:CD	2.34	0.53
1:B:81:LEU:HA	1:B:84:LEU:HD12	1.89	0.53
1:D:91:ARG:HG2	1:D:215:MET:SD	2.48	0.53
1:D:16:LEU:HD22	1:D:63:ILE:HD11	1.89	0.52
1:D:24:VAL:HB	1:D:67:THR:HG23	1.91	0.52
1:F:165:GLY:O	1:F:167:GLU:N	2.42	0.52
1:A:34:ILE:HA	1:A:37:LEU:HD23	1.90	0.52
1:B:5:ASP:CB	1:B:12:THR:HA	2.36	0.52
1:B:35:ALA:C	1:B:37:LEU:H	2.17	0.52
1:B:116:LEU:HB2	1:B:158:SER:O	2.10	0.52
1:D:71:GLY:N	1:D:72:PRO:CD	2.72	0.52
1:E:13:LYS:HE3	1:E:84:LEU:O	2.08	0.52
1:E:40:LYS:HE2	1:F:142:GLU:OE2	2.09	0.52
1:E:185:GLU:O	1:E:188:GLN:HB2	2.10	0.52
1:A:161:THR:HG22	1:F:119:ALA:HB1	1.91	0.52
1:B:26:GLY:HA2	1:B:67:THR:OG1	2.09	0.52
1:C:35:ALA:HA	1:C:38:MET:HE2	1.90	0.52
1:D:28:PRO:HB3	1:D:51:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:NH1	1:D:128:PHE:O	2.41	0.52
1:E:162:PHE:O	1:E:166:GLN:HB2	2.10	0.52
1:F:151:THR:CG2	1:F:152:HIS:N	2.73	0.52
1:A:49:GLU:HG2	1:F:49:GLU:HG2	1.92	0.52
1:B:62:VAL:CG2	1:B:253:LEU:HD11	2.39	0.52
1:C:235:LYS:HA	1:C:238:GLU:OE2	2.09	0.52
1:D:164:PRO:O	1:D:176:VAL:HG13	2.09	0.52
1:C:95:THR:O	1:C:220:ILE:HG22	2.09	0.52
1:F:6:VAL:CG2	1:F:10:GLY:H	2.22	0.52
1:A:156:THR:CG2	1:A:157:ALA:H	2.18	0.52
1:A:163:TYR:HA	1:A:168:ARG:HD2	1.90	0.52
1:B:212:ARG:NH2	1:B:252:LEU:HB3	2.25	0.52
1:D:188:GLN:O	1:D:190:MET:N	2.43	0.52
1:D:219:VAL:HG12	1:D:221:VAL:O	2.10	0.52
1:E:26:GLY:O	1:E:27:ASP:HB2	2.09	0.52
1:E:56:GLU:HA	1:E:60:LYS:O	2.09	0.52
1:F:243:LYS:O	1:F:247:GLU:HB2	2.10	0.52
1:B:43:LYS:HB2	1:B:53:TRP:CH2	2.44	0.52
1:D:133:ASP:CB	1:D:212:ARG:HG2	2.38	0.52
1:E:206:CYS:HB3	1:E:211:LEU:O	2.08	0.52
1:A:105:GLY:H	1:A:219:VAL:HB	1.75	0.52
1:D:151:THR:CG2	1:D:152:HIS:N	2.72	0.52
1:E:25:PRO:HB3	1:E:92:ILE:HG23	1.92	0.52
1:E:126:MET:O	1:E:126:MET:HG3	2.08	0.52
1:B:15:ASP:O	1:B:54:ARG:NH1	2.42	0.52
1:D:138:THR:O	1:D:142:GLU:HG3	2.10	0.52
1:F:230:ASN:O	1:F:234:MET:SD	2.68	0.52
1:B:69:ILE:H	1:B:69:ILE:CD1	2.22	0.52
1:D:187:TRP:HA	1:D:187:TRP:HE3	1.75	0.52
1:F:17:GLN:HE21	1:F:17:GLN:HA	1.74	0.52
1:F:103:ASN:HB2	1:F:106:ASP:OD1	2.08	0.52
1:A:108:LEU:CD1	1:A:194:ASN:HB3	2.39	0.51
1:B:133:ASP:OD2	1:B:135:ALA:HB3	2.09	0.51
1:D:206:CYS:SG	1:D:213:ALA:HB2	2.50	0.51
1:E:161:THR:O	1:E:166:GLN:HG3	2.11	0.51
1:B:81:LEU:HD12	1:B:89:PHE:HE2	1.74	0.51
1:B:92:ILE:CD1	1:B:241:ALA:HB1	2.40	0.51
1:D:36:ALA:O	1:D:37:LEU:HG	2.10	0.51
1:D:162:PHE:O	1:D:166:GLN:HG3	2.10	0.51
1:D:179:ARG:HH11	1:D:179:ARG:CB	2.20	0.51
1:E:81:LEU:HD22	1:E:86:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:CYS:O	1:A:66:SER:C	2.53	0.51
1:C:112:ALA:HA	1:C:130:ALA:O	2.10	0.51
1:B:105:GLY:O	1:B:106:ASP:C	2.54	0.51
1:A:226:GLN:CD	1:A:227:GLU:N	2.69	0.51
1:B:28:PRO:HG3	1:B:49:GLU:OE1	2.11	0.51
1:E:58:ASP:O	1:E:60:LYS:HG2	2.10	0.51
1:A:162:PHE:O	1:A:166:GLN:HG3	2.10	0.51
1:B:103:ASN:HB2	1:B:106:ASP:OD1	2.11	0.51
1:B:152:HIS:HB2	1:B:193:MET:HE3	1.92	0.51
1:D:137:THR:O	1:D:137:THR:HG22	2.11	0.51
1:E:8:HIS:HB3	1:E:50:PHE:HE1	1.70	0.51
1:F:187:TRP:O	1:F:192:VAL:HG23	2.10	0.51
1:F:199:SER:O	1:F:200:ALA:C	2.54	0.51
1:A:5:ASP:OD1	1:A:12:THR:HA	2.11	0.51
1:A:8:HIS:H	1:A:8:HIS:HD1	1.53	0.51
1:C:5:ASP:OD1	1:C:12:THR:HA	2.11	0.51
1:D:38:MET:HG2	1:D:57:LEU:HD13	1.93	0.51
1:D:76:ILE:HG22	1:D:80:GLU:CG	2.36	0.51
1:E:29:GLU:O	1:E:33:LYS:HG2	2.11	0.51
1:F:57:LEU:HB3	1:F:253:LEU:HD11	1.92	0.51
1:F:161:THR:O	1:F:166:GLN:HG2	2.11	0.51
1:F:176:VAL:HB	1:F:180:PHE:HB2	1.93	0.51
1:E:21:LEU:HD22	1:E:62:VAL:HG13	1.93	0.51
1:E:54:ARG:HG2	1:E:54:ARG:HH11	1.74	0.51
2:B:254:ACY:CH3	1:D:48:ARG:HH12	2.18	0.51
1:F:151:THR:HG23	1:F:152:HIS:N	2.26	0.51
1:F:156:THR:HG23	1:F:194:ASN:CG	2.36	0.51
1:F:159:SER:HB3	1:F:166:GLN:NE2	2.25	0.51
1:A:7:PHE:O	1:A:8:HIS:C	2.54	0.50
1:B:57:LEU:CG	1:B:250:ARG:HG2	2.41	0.50
1:B:236:GLN:HA	1:B:239:SER:OG	2.11	0.50
1:C:31:VAL:HG21	1:C:51:THR:HB	1.93	0.50
1:F:48:ARG:HG2	1:F:48:ARG:HH11	1.75	0.50
1:F:154:GLY:C	1:F:193:MET:HE2	2.36	0.50
1:D:178:ARG:HG3	1:D:178:ARG:HH11	1.76	0.50
1:E:160:ASP:O	1:E:161:THR:HG23	2.12	0.50
1:A:177:VAL:HG22	1:A:178:ARG:N	2.26	0.50
1:C:158:SER:HB2	1:C:199:SER:OG	2.11	0.50
1:E:97:ALA:O	1:E:222:ASN:ND2	2.44	0.50
1:F:16:LEU:HD22	1:F:63:ILE:HG13	1.92	0.50
1:F:98:ILE:HD12	1:F:195:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:ALA:N	1:F:251:ARG:NH1	2.51	0.50
1:A:106:ASP:HB2	1:A:219:VAL:HG21	1.93	0.50
1:B:96:GLY:HA2	1:B:221:VAL:O	2.11	0.50
1:D:156:THR:HG23	1:D:194:ASN:HD21	1.77	0.50
1:F:113:SER:H	1:F:130:ALA:HB3	1.77	0.50
1:F:196:GLU:OE2	1:F:197:MET:C	2.54	0.50
1:F:199:SER:O	1:F:200:ALA:O	2.30	0.50
1:A:37:LEU:N	1:A:37:LEU:CD2	2.75	0.50
1:A:156:THR:CG2	1:A:157:ALA:N	2.74	0.50
1:C:28:PRO:HB2	1:C:51:THR:OG1	2.12	0.50
1:F:163:TYR:CA	1:F:168:ARG:HD2	2.38	0.50
1:B:142:GLU:OE2	1:E:42:VAL:HG13	2.11	0.50
1:B:186:GLU:CG	1:B:190:MET:HE3	2.41	0.50
1:C:22:ALA:HB2	1:C:86:ILE:HD13	1.94	0.50
1:F:21:LEU:HD13	1:F:253:LEU:CD2	2.40	0.50
1:B:124:ALA:HA	1:D:175:ARG:NE	2.24	0.50
1:B:124:ALA:N	1:D:175:ARG:HE	2.09	0.50
1:C:225:GLN:HG2	1:C:226:GLN:N	2.26	0.50
1:D:140:LEU:HD23	1:D:248:ALA:CB	2.42	0.50
1:D:188:GLN:O	1:D:191:GLY:N	2.45	0.50
1:E:81:LEU:HB3	1:E:86:ILE:HD12	1.94	0.50
1:F:200:ALA:O	1:F:201:THR:C	2.55	0.50
1:A:178:ARG:CA	1:A:181:LYS:HE2	2.42	0.50
1:B:81:LEU:HA	1:B:84:LEU:CD1	2.42	0.50
1:B:169:TYR:CE2	1:B:176:VAL:HG23	2.47	0.50
1:E:147:ILE:HD13	1:E:148:GLY:N	2.27	0.50
1:F:117:ASP:CG	1:F:118:GLY:N	2.69	0.50
1:F:236:GLN:HA	1:F:239:SER:HG	1.75	0.50
1:B:230:ASN:O	1:B:234:MET:HE1	2.11	0.49
1:E:25:PRO:HG3	1:E:34:ILE:HD12	1.94	0.49
1:E:57:LEU:O	1:E:60:LYS:HB2	2.11	0.49
1:A:201:THR:O	1:A:205:MET:CB	2.60	0.49
1:B:40:LYS:N	1:B:41:PRO:CD	2.74	0.49
1:C:123:PHE:HA	1:E:175:ARG:NH2	2.27	0.49
1:C:140:LEU:HD22	1:C:216:VAL:HB	1.93	0.49
1:E:156:THR:CG2	1:E:194:ASN:ND2	2.74	0.49
1:E:161:THR:HG1	1:E:165:GLY:HA3	1.75	0.49
1:F:95:THR:OG1	1:F:96:GLY:N	2.45	0.49
1:A:35:ALA:HA	1:A:38:MET:CE	2.41	0.49
1:B:164:PRO:HG2	1:B:165:GLY:N	2.26	0.49
1:B:190:MET:HE1	1:F:125:PRO:CD	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:THR:HG22	1:C:205:MET:CE	2.23	0.49
1:E:94:THR:HG21	1:E:238:GLU:HG2	1.93	0.49
1:F:227:GLU:CG	1:F:228:ILE:N	2.75	0.49
1:A:92:ILE:HD13	1:A:93:GLY:N	2.28	0.49
1:B:95:THR:OG1	1:B:194:ASN:HB2	2.12	0.49
1:B:196:GLU:OE2	1:B:199:SER:N	2.46	0.49
1:C:95:THR:OG1	1:C:96:GLY:N	2.45	0.49
1:D:27:ASP:HB2	1:D:28:PRO:HD2	1.94	0.49
1:B:56:GLU:OE2	1:C:43:LYS:NZ	2.46	0.49
1:B:243:LYS:O	1:B:246:VAL:HB	2.13	0.49
1:B:243:LYS:O	1:B:246:VAL:N	2.42	0.49
1:C:172:TYR:CE1	1:E:211:LEU:HD21	2.47	0.49
1:E:238:GLU:O	1:E:242:VAL:HG23	2.12	0.49
1:F:146:SER:HB3	1:F:251:ARG:HH22	1.77	0.49
1:A:222:ASN:OD1	1:A:225:GLN:HB2	2.12	0.49
1:E:4:SER:O	1:E:5:ASP:CG	2.56	0.49
1:E:15:ASP:CB	1:E:44:LEU:HD21	2.43	0.49
1:E:79:GLU:C	1:E:83:GLN:NE2	2.71	0.49
1:F:236:GLN:O	1:F:237:THR:C	2.55	0.49
1:C:105:GLY:HA3	1:C:236:GLN:NE2	2.28	0.49
1:C:135:ALA:O	1:C:252:LEU:HD21	2.12	0.49
1:C:242:VAL:O	1:C:245:VAL:HG12	2.13	0.49
1:E:16:LEU:HB3	1:E:19:ALA:HB3	1.93	0.49
1:B:232:GLU:O	1:B:236:GLN:N	2.24	0.49
1:C:161:THR:OG1	1:C:164:PRO:HG2	2.12	0.49
1:E:142:GLU:O	1:E:145:LYS:N	2.44	0.49
1:B:31:VAL:CG1	1:B:53:TRP:HB2	2.42	0.49
1:D:17:GLN:HA	1:D:17:GLN:NE2	2.21	0.49
1:B:232:GLU:C	1:B:234:MET:H	2.21	0.49
1:C:196:GLU:OE1	1:C:215:MET:SD	2.71	0.49
1:F:163:TYR:N	1:F:164:PRO:HD2	2.28	0.49
1:D:34:ILE:HG22	1:D:38:MET:HE1	1.94	0.48
1:E:237:THR:HA	1:E:240:HIS:HD2	1.75	0.48
1:F:94:THR:HB	1:F:220:ILE:HG23	1.93	0.48
1:F:107:VAL:C	1:F:108:LEU:HD23	2.38	0.48
1:F:144:ALA:HA	1:F:244:ILE:CD1	2.43	0.48
1:A:92:ILE:HG13	1:A:241:ALA:O	2.13	0.48
1:A:140:LEU:HD23	1:A:248:ALA:HB1	1.94	0.48
1:A:142:GLU:O	1:A:145:LYS:HB2	2.13	0.48
1:B:236:GLN:C	1:B:238:GLU:N	2.66	0.48
1:C:31:VAL:HG13	1:C:64:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:ALA:HA	1:E:244:ILE:HD12	1.95	0.48
1:E:163:TYR:HB2	1:E:164:PRO:CD	2.42	0.48
1:E:163:TYR:HB2	1:E:164:PRO:HD3	1.94	0.48
1:B:8:HIS:HB3	1:B:50:PHE:HE1	1.76	0.48
1:B:48:ARG:NH1	1:D:49:GLU:OE1	2.46	0.48
1:B:105:GLY:H	1:B:219:VAL:HB	1.78	0.48
1:C:187:TRP:HB3	1:C:192:VAL:HG21	1.94	0.48
1:C:233:THR:HA	1:C:236:GLN:OE1	2.13	0.48
1:E:78:VAL:HA	1:E:81:LEU:HD12	1.94	0.48
1:A:238:GLU:O	1:A:242:VAL:HG23	2.12	0.48
1:E:187:TRP:HA	1:E:190:MET:HE3	1.94	0.48
1:F:96:GLY:HA3	1:F:223:ARG:HG2	1.96	0.48
1:A:73:SER:O	1:A:74:THR:C	2.56	0.48
1:C:25:PRO:O	1:C:66:SER:HA	2.13	0.48
1:D:47:HIS:O	1:D:48:ARG:C	2.56	0.48
1:E:16:LEU:HD23	1:E:16:LEU:N	2.28	0.48
1:F:158:SER:OG	1:F:200:ALA:HB2	2.12	0.48
1:A:6:VAL:HG23	1:A:6:VAL:O	2.13	0.48
1:B:238:GLU:O	1:B:239:SER:C	2.57	0.48
1:C:109:VAL:O	1:C:193:MET:HE1	2.12	0.48
1:A:120:SER:HB2	1:A:204:THR:HG21	1.96	0.48
1:B:5:ASP:HB2	1:B:12:THR:CA	2.41	0.48
1:D:41:PRO:HA	1:D:54:ARG:O	2.14	0.48
1:D:156:THR:CG2	1:D:194:ASN:HD21	2.26	0.48
1:E:91:ARG:HG3	1:E:92:ILE:H	1.74	0.48
1:E:175:ARG:C	1:E:175:ARG:HH11	2.21	0.48
1:E:176:VAL:CG1	1:E:180:PHE:HB3	2.43	0.48
1:F:98:ILE:HD11	1:F:194:ASN:HA	1.96	0.48
1:A:97:ALA:HA	1:A:193:MET:O	2.14	0.48
1:C:121:LEU:O	1:E:177:VAL:HG21	2.14	0.48
1:D:58:ASP:OD2	1:D:58:ASP:N	2.44	0.48
1:E:57:LEU:CD2	1:E:250:ARG:HG2	2.39	0.48
1:E:177:VAL:O	1:E:178:ARG:C	2.56	0.48
1:E:236:GLN:O	1:E:239:SER:N	2.42	0.48
1:F:183:SER:HB2	1:F:187:TRP:NE1	2.29	0.48
1:A:8:HIS:ND1	1:A:8:HIS:N	2.52	0.48
1:A:177:VAL:HG22	1:A:178:ARG:H	1.79	0.48
1:B:5:ASP:HB2	1:B:11:LEU:O	2.14	0.48
1:B:35:ALA:C	1:B:37:LEU:N	2.71	0.48
1:C:187:TRP:C	1:C:189:ALA:H	2.20	0.48
1:A:9:LEU:HD23	1:A:50:PHE:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLU:HG2	1:A:57:LEU:N	2.29	0.48
1:A:114:VAL:HG23	1:A:156:THR:O	2.13	0.48
1:A:158:SER:CB	1:A:200:ALA:HB2	2.44	0.48
1:B:236:GLN:OE1	1:B:236:GLN:O	2.32	0.48
1:D:126:MET:HG3	1:D:126:MET:O	2.13	0.48
1:E:17:GLN:CG	1:E:54:ARG:HH21	2.17	0.48
1:F:27:ASP:OD1	1:F:28:PRO:HD2	2.14	0.48
1:B:127:GLU:HG3	1:F:126:MET:HE2	1.95	0.47
1:B:144:ALA:HA	1:B:244:ILE:HG12	1.95	0.47
1:B:164:PRO:O	1:B:166:GLN:N	2.46	0.47
1:C:78:VAL:HG13	1:C:89:PHE:CE2	2.48	0.47
1:C:239:SER:O	1:C:243:LYS:HB2	2.13	0.47
1:D:133:ASP:OD2	1:D:135:ALA:N	2.47	0.47
1:D:238:GLU:C	1:D:238:GLU:OE2	2.57	0.47
1:E:17:GLN:HE21	1:E:17:GLN:CA	2.10	0.47
1:E:54:ARG:HH11	1:E:54:ARG:CG	2.27	0.47
1:B:78:VAL:HG21	1:B:205:MET:CE	2.43	0.47
1:C:205:MET:HG3	1:C:206:CYS:N	2.28	0.47
1:D:16:LEU:HD11	1:D:84:LEU:CB	2.44	0.47
1:E:91:ARG:HG2	1:E:215:MET:HG2	1.95	0.47
1:E:147:ILE:HD13	1:E:149:ALA:N	2.29	0.47
1:F:57:LEU:HD11	1:F:250:ARG:HH12	1.74	0.47
1:A:143:ALA:HB1	1:A:247:GLU:HG3	1.95	0.47
1:C:172:TYR:HE1	1:E:211:LEU:HD21	1.79	0.47
1:E:114:VAL:HB	1:E:157:ALA:HA	1.96	0.47
1:F:183:SER:O	1:F:184:MET:C	2.55	0.47
1:F:5:ASP:CB	1:F:12:THR:HA	2.44	0.47
1:F:176:VAL:HG12	1:F:177:VAL:N	2.28	0.47
1:B:149:ALA:HB2	1:B:244:ILE:HD11	1.95	0.47
1:C:163:TYR:CD2	1:C:171:THR:HG22	2.48	0.47
1:D:146:SER:O	1:D:148:GLY:N	2.46	0.47
1:F:221:VAL:HG22	1:F:223:ARG:H	1.80	0.47
1:A:93:GLY:O	1:A:217:ALA:HA	2.13	0.47
1:A:178:ARG:HA	1:A:181:LYS:HG3	1.96	0.47
1:B:23:ILE:C	1:B:24:VAL:HG13	2.40	0.47
1:C:21:LEU:O	1:C:22:ALA:HB2	2.14	0.47
1:C:132:ALA:HA	1:C:203:LEU:CD2	2.44	0.47
1:D:91:ARG:HG3	1:D:91:ARG:HH11	1.80	0.47
1:D:115:ARG:NH2	1:D:124:ALA:O	2.45	0.47
1:D:188:GLN:C	1:D:190:MET:N	2.73	0.47
1:E:63:ILE:CG2	1:E:64:VAL:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:GLU:O	1:E:83:GLN:NE2	2.48	0.47
1:F:116:LEU:HD21	1:F:187:TRP:CH2	2.50	0.47
1:F:250:ARG:O	1:F:253:LEU:HB2	2.15	0.47
1:F:91:ARG:O	1:F:216:VAL:HG12	2.14	0.47
1:F:99:GLN:HB3	1:F:101:HIS:ND1	2.30	0.47
1:E:7:PHE:O	1:E:8:HIS:C	2.58	0.47
1:E:39:ASP:O	1:E:56:GLU:HB3	2.15	0.47
1:F:9:LEU:HD21	1:F:77:ALA:HA	1.95	0.47
1:F:96:GLY:HA2	1:F:221:VAL:O	2.15	0.47
1:B:119:ALA:O	1:B:122:HIS:HB2	2.15	0.47
1:C:163:TYR:HA	1:C:168:ARG:HD2	1.97	0.47
1:D:38:MET:HG2	1:D:57:LEU:CD1	2.45	0.47
1:D:172:TYR:O	1:D:173:SER:C	2.57	0.47
1:D:174:GLY:O	1:D:175:ARG:C	2.58	0.47
1:F:198:GLU:H	1:F:198:GLU:CD	2.23	0.47
1:C:250:ARG:O	1:C:253:LEU:HB2	2.14	0.46
1:E:91:ARG:HB3	1:E:215:MET:HG2	1.97	0.46
1:B:33:LYS:HA	1:B:33:LYS:CE	2.32	0.46
1:B:151:THR:HG22	1:B:152:HIS:N	2.30	0.46
1:D:34:ILE:O	1:D:35:ALA:C	2.58	0.46
1:E:149:ALA:O	1:E:151:THR:N	2.49	0.46
1:F:17:GLN:HE21	1:F:17:GLN:CA	2.28	0.46
1:F:110:THR:HA	1:F:154:GLY:O	2.15	0.46
1:C:18:GLY:O	1:C:19:ALA:C	2.58	0.46
1:C:63:ILE:CG2	1:C:64:VAL:N	2.77	0.46
1:C:180:PHE:HE1	1:E:122:HIS:CG	2.33	0.46
1:E:92:ILE:CG1	1:E:93:GLY:N	2.78	0.46
1:E:199:SER:CB	1:E:215:MET:HE2	2.44	0.46
1:E:226:GLN:O	1:E:227:GLU:C	2.59	0.46
1:F:185:GLU:CD	1:F:185:GLU:C	2.83	0.46
1:A:73:SER:O	1:A:76:ILE:N	2.49	0.46
1:A:131:VAL:CG2	1:A:132:ALA:N	2.78	0.46
1:B:83:GLN:NE2	1:D:171:THR:HG23	2.30	0.46
1:B:107:VAL:O	1:B:151:THR:HA	2.16	0.46
1:C:44:LEU:HB2	1:C:52:SER:O	2.15	0.46
1:C:113:SER:O	1:C:130:ALA:HB3	2.15	0.46
1:C:233:THR:HA	1:C:236:GLN:CG	2.45	0.46
1:F:133:ASP:CG	1:F:212:ARG:HG2	2.41	0.46
1:A:39:ASP:O	1:A:40:LYS:C	2.57	0.46
1:A:43:LYS:HB2	1:A:53:TRP:CH2	2.50	0.46
1:C:96:GLY:HA2	1:C:221:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:GLU:OE2	1:D:83:GLN:HG3	2.16	0.46
1:E:39:ASP:O	1:E:40:LYS:CB	2.62	0.46
1:E:57:LEU:O	1:E:58:ASP:C	2.57	0.46
1:E:172:TYR:C	1:E:172:TYR:CD2	2.94	0.46
1:A:178:ARG:O	1:A:180:PHE:N	2.49	0.46
1:C:11:LEU:HD21	1:C:52:SER:OG	2.15	0.46
1:D:21:LEU:HD21	1:D:90:LEU:HD11	1.98	0.46
1:E:44:LEU:O	1:E:45:ALA:HB2	2.16	0.46
1:F:34:ILE:CD1	1:F:242:VAL:HG22	2.45	0.46
1:A:234:MET:O	1:A:237:THR:HB	2.15	0.46
1:B:69:ILE:HG21	1:D:76:ILE:HD11	1.97	0.46
1:C:62:VAL:HG13	1:C:63:ILE:N	2.31	0.46
1:C:233:THR:HA	1:C:236:GLN:CD	2.40	0.46
1:D:230:ASN:HD22	1:D:232:GLU:HB3	1.81	0.46
1:E:31:VAL:HG13	1:E:64:VAL:CG1	2.36	0.46
1:F:71:GLY:N	1:F:72:PRO:CD	2.79	0.46
1:F:168:ARG:C	1:F:170:ASP:H	2.24	0.46
1:D:175:ARG:HH12	1:D:178:ARG:H	1.64	0.46
1:D:222:ASN:ND2	1:D:225:GLN:HG2	2.30	0.46
1:E:6:VAL:HG11	1:E:84:LEU:HG	1.96	0.46
1:E:81:LEU:O	1:E:84:LEU:HB2	2.15	0.46
1:F:24:VAL:O	1:F:24:VAL:HG23	2.16	0.46
1:A:75:SER:O	1:A:79:GLU:HB3	2.15	0.46
1:B:44:LEU:HD11	1:B:54:ARG:HB2	1.96	0.46
1:B:156:THR:HG21	1:B:196:GLU:HG2	1.98	0.46
1:C:38:MET:CG	1:C:57:LEU:HD13	2.40	0.46
1:C:233:THR:CA	1:C:236:GLN:HG3	2.46	0.46
1:E:36:ALA:C	1:E:38:MET:H	2.23	0.46
1:B:236:GLN:O	1:B:239:SER:N	2.49	0.46
1:D:86:ILE:CD1	1:D:86:ILE:N	2.78	0.46
1:D:86:ILE:N	1:D:86:ILE:HD12	2.31	0.46
1:D:168:ARG:HH11	1:D:223:ARG:NH1	2.13	0.46
1:D:177:VAL:HG22	1:D:179:ARG:N	2.23	0.46
1:E:8:HIS:CB	1:E:50:PHE:CE1	2.96	0.46
1:E:39:ASP:HA	1:F:145:LYS:HE3	1.98	0.46
1:F:107:VAL:HG23	1:F:217:ALA:O	2.16	0.46
1:A:247:GLU:OE1	1:A:250:ARG:HD2	2.16	0.45
1:B:164:PRO:C	1:B:166:GLN:N	2.68	0.45
1:D:25:PRO:HD2	1:D:65:CYS:O	2.15	0.45
1:D:107:VAL:HG23	1:D:151:THR:HA	1.97	0.45
1:E:161:THR:HB	1:E:165:GLY:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:GLU:CD	1:E:198:GLU:H	2.24	0.45
1:A:90:LEU:HD22	1:A:140:LEU:HD21	1.97	0.45
1:B:236:GLN:O	1:B:239:SER:HB2	2.17	0.45
1:C:23:ILE:HA	1:C:90:LEU:O	2.16	0.45
1:C:45:ALA:O	1:C:46:SER:HB2	2.16	0.45
1:C:169:TYR:C	1:C:171:THR:N	2.74	0.45
1:D:55:ALA:O	1:D:56:GLU:HG3	2.17	0.45
1:D:245:VAL:CG1	1:D:246:VAL:N	2.79	0.45
1:E:114:VAL:HG12	1:E:116:LEU:HG	1.99	0.45
1:A:24:VAL:HB	1:A:67:THR:HG23	1.98	0.45
1:B:82:ALA:O	1:B:85:GLY:N	2.49	0.45
1:B:98:ILE:HG13	1:B:99:GLN:N	2.30	0.45
1:D:98:ILE:O	1:D:188:GLN:NE2	2.49	0.45
1:D:172:TYR:O	1:D:172:TYR:HD1	1.99	0.45
1:F:230:ASN:CG	1:F:231:ALA:N	2.74	0.45
1:A:164:PRO:O	1:A:165:GLY:C	2.59	0.45
1:A:242:VAL:O	1:A:245:VAL:HG12	2.16	0.45
1:B:120:SER:HB2	1:B:204:THR:HG21	1.99	0.45
1:D:6:VAL:HG22	1:D:11:LEU:O	2.17	0.45
1:D:89:PHE:N	1:D:212:ARG:O	2.48	0.45
1:D:158:SER:CB	1:D:200:ALA:HB2	2.46	0.45
1:D:136:CYS:HA	1:D:252:LEU:HD11	1.98	0.45
1:E:19:ALA:HB2	1:E:61:ALA:HB1	1.99	0.45
1:A:233:THR:O	1:A:234:MET:HB2	2.17	0.45
1:B:54:ARG:HG2	1:B:55:ALA:N	2.31	0.45
1:A:49:GLU:O	1:A:51:THR:N	2.50	0.45
1:B:28:PRO:O	1:B:31:VAL:HG23	2.17	0.45
1:B:34:ILE:HB	1:B:64:VAL:HG11	1.99	0.45
1:B:162:PHE:CD1	1:B:162:PHE:C	2.95	0.45
1:C:9:LEU:CD1	1:C:81:LEU:HG	2.45	0.45
1:C:143:ALA:HB1	1:C:247:GLU:HB3	1.99	0.45
1:C:201:THR:O	1:C:205:MET:HE2	2.17	0.45
1:E:210:GLY:O	1:E:211:LEU:HD23	2.15	0.45
1:F:159:SER:CB	1:F:166:GLN:NE2	2.79	0.45
1:F:198:GLU:N	1:F:198:GLU:CD	2.74	0.45
1:B:128:PHE:CD1	1:B:129:PRO:N	2.85	0.45
1:B:142:GLU:O	1:B:145:LYS:N	2.49	0.45
1:C:44:LEU:CD1	1:C:54:ARG:HB2	2.41	0.45
1:E:194:ASN:N	1:E:194:ASN:ND2	2.47	0.45
1:F:80:GLU:O	1:F:84:LEU:HG	2.17	0.45
1:A:226:GLN:CD	1:A:227:GLU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:O	1:A:250:ARG:CB	2.65	0.45
1:C:13:LYS:HG3	1:C:84:LEU:O	2.17	0.45
1:C:139:ALA:O	1:C:142:GLU:N	2.50	0.45
1:C:216:VAL:HG22	1:C:217:ALA:N	2.32	0.45
1:D:56:GLU:HG2	1:D:61:ALA:HA	1.98	0.45
1:E:44:LEU:HB2	1:E:53:TRP:C	2.42	0.45
1:E:236:GLN:O	1:E:237:THR:C	2.60	0.45
1:E:245:VAL:HG13	1:E:246:VAL:N	2.32	0.45
1:E:250:ARG:HA	1:E:253:LEU:HD12	1.97	0.45
1:B:99:GLN:NE2	1:B:191:GLY:HA2	2.32	0.45
1:B:201:THR:HG22	1:B:205:MET:HE2	1.99	0.45
1:D:17:GLN:NE2	1:D:17:GLN:CA	2.80	0.45
1:D:118:GLY:O	1:D:122:HIS:CD2	2.70	0.45
1:D:196:GLU:OE2	1:D:199:SER:OG	2.30	0.45
1:D:228:ILE:N	1:D:228:ILE:CD1	2.76	0.45
1:D:228:ILE:H	1:D:228:ILE:CD1	2.30	0.45
1:A:56:GLU:HG2	1:A:60:LYS:O	2.16	0.44
1:B:60:LYS:CB	1:B:253:LEU:HD22	2.46	0.44
1:B:162:PHE:O	1:B:162:PHE:CD1	2.70	0.44
1:B:184:MET:CE	1:B:188:GLN:NE2	2.80	0.44
1:D:112:ALA:HA	1:D:130:ALA:O	2.17	0.44
1:F:23:ILE:O	1:F:64:VAL:HA	2.16	0.44
1:F:28:PRO:HA	1:F:66:SER:HB3	1.98	0.44
1:F:149:ALA:O	1:F:151:THR:N	2.47	0.44
1:F:177:VAL:HG22	1:F:178:ARG:N	2.27	0.44
1:C:31:VAL:HG11	1:C:51:THR:HG22	1.99	0.44
1:C:92:ILE:HD13	1:C:93:GLY:N	2.32	0.44
1:C:223:ARG:O	1:C:225:GLN:O	2.35	0.44
1:D:91:ARG:HG3	1:D:91:ARG:NH1	2.32	0.44
1:D:146:SER:C	1:D:148:GLY:N	2.75	0.44
1:E:180:PHE:O	1:E:181:LYS:C	2.60	0.44
1:F:37:LEU:HD22	1:F:242:VAL:CG1	2.47	0.44
1:A:173:SER:OG	1:F:209:GLN:NE2	2.49	0.44
1:C:91:ARG:HG3	1:C:91:ARG:HH11	1.82	0.44
1:D:12:THR:H	1:D:15:ASP:CG	2.23	0.44
1:D:78:VAL:O	1:D:81:LEU:N	2.50	0.44
1:E:21:LEU:HA	1:E:86:ILE:HG23	1.98	0.44
1:F:120:SER:HB2	1:F:204:THR:HG21	1.99	0.44
1:A:71:GLY:N	1:A:72:PRO:CD	2.80	0.44
1:A:147:ILE:HD12	1:A:147:ILE:O	2.17	0.44
1:A:173:SER:HB3	1:F:209:GLN:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLU:HA	1:B:60:LYS:O	2.17	0.44
1:C:75:SER:O	1:C:79:GLU:HB3	2.16	0.44
1:C:202:LEU:HA	1:C:205:MET:HE3	1.99	0.44
1:D:171:THR:C	1:D:173:SER:N	2.73	0.44
1:D:178:ARG:HG3	1:D:178:ARG:NH1	2.32	0.44
1:E:140:LEU:HD13	1:E:216:VAL:HB	1.98	0.44
1:F:35:ALA:C	1:F:37:LEU:H	2.25	0.44
1:F:183:SER:HB2	1:F:187:TRP:HE1	1.81	0.44
1:B:182:GLY:O	1:B:185:GLU:HB3	2.17	0.44
1:C:38:MET:HA	1:C:57:LEU:HD13	2.00	0.44
1:C:94:THR:HG22	1:C:220:ILE:HB	1.98	0.44
1:C:187:TRP:HA	1:C:187:TRP:CE3	2.52	0.44
1:E:91:ARG:CG	1:E:92:ILE:N	2.77	0.44
1:A:16:LEU:HD13	1:A:63:ILE:HD12	2.00	0.44
1:C:91:ARG:NH1	1:C:91:ARG:HG3	2.33	0.44
1:C:173:SER:CB	1:E:209:GLN:HE21	2.30	0.44
1:D:206:CYS:O	1:D:209:GLN:N	2.49	0.44
1:D:210:GLY:O	1:D:211:LEU:HD23	2.18	0.44
1:F:144:ALA:CA	1:F:244:ILE:HD12	2.48	0.44
1:A:225:GLN:HG2	1:A:226:GLN:H	1.83	0.44
1:B:40:LYS:N	1:B:41:PRO:HD3	2.32	0.44
1:B:108:LEU:HD11	1:B:219:VAL:HG22	2.00	0.44
1:C:38:MET:HB2	1:C:55:ALA:CB	2.47	0.44
1:C:163:TYR:O	1:C:168:ARG:HB2	2.18	0.44
1:D:94:THR:CG2	1:D:220:ILE:HG23	2.47	0.44
1:E:162:PHE:HB3	1:E:163:TYR:H	1.72	0.44
1:A:6:VAL:HB	1:A:80:GLU:CD	2.41	0.44
1:B:98:ILE:HD11	1:B:192:VAL:C	2.42	0.44
1:B:143:ALA:HB1	1:B:247:GLU:HB3	2.00	0.44
1:D:188:GLN:C	1:D:190:MET:H	2.26	0.44
1:E:161:THR:HB	1:E:165:GLY:N	2.33	0.44
1:F:8:HIS:CG	1:F:76:ILE:HG21	2.52	0.44
1:A:74:THR:O	1:A:75:SER:C	2.61	0.44
1:A:180:PHE:O	1:A:183:SER:N	2.46	0.44
1:A:236:GLN:HA	1:A:239:SER:OG	2.17	0.44
1:B:160:ASP:O	1:D:72:PRO:HB3	2.17	0.44
1:C:88:THR:OG1	1:C:212:ARG:HB2	2.18	0.44
1:C:122:HIS:O	1:E:175:ARG:NH2	2.51	0.44
1:C:187:TRP:HA	1:C:187:TRP:HE3	1.82	0.44
1:D:19:ALA:HB2	1:D:61:ALA:CB	2.48	0.44
1:D:24:VAL:HB	1:D:67:THR:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ASN:ND2	1:D:225:GLN:OE1	2.51	0.44
1:E:247:GLU:OE2	1:E:250:ARG:CZ	2.65	0.44
1:F:57:LEU:HD23	1:F:253:LEU:HD11	1.99	0.44
1:F:142:GLU:O	1:F:146:SER:N	2.43	0.44
1:A:223:ARG:C	1:A:225:GLN:N	2.76	0.43
1:B:206:CYS:O	1:B:207:ALA:C	2.59	0.43
1:C:187:TRP:O	1:C:189:ALA:N	2.39	0.43
1:E:8:HIS:HB3	1:E:50:PHE:HD1	1.82	0.43
1:E:175:ARG:HD2	1:E:176:VAL:C	2.44	0.43
1:E:177:VAL:HG12	1:E:180:PHE:HB2	1.99	0.43
1:A:63:ILE:HG22	1:A:64:VAL:N	2.32	0.43
1:A:96:GLY:HA2	1:A:221:VAL:O	2.18	0.43
1:E:19:ALA:HA	1:E:61:ALA:HB3	2.01	0.43
1:E:93:GLY:O	1:E:217:ALA:CA	2.64	0.43
1:F:250:ARG:HA	1:F:253:LEU:HD12	1.98	0.43
1:B:40:LYS:HD2	1:B:56:GLU:CB	2.48	0.43
1:B:91:ARG:HH22	2:B:254:ACY:C	2.30	0.43
1:C:71:GLY:N	1:C:72:PRO:CD	2.81	0.43
1:E:37:LEU:HD22	1:E:37:LEU:HA	1.84	0.43
1:E:115:ARG:HH12	1:E:126:MET:HA	1.80	0.43
1:A:48:ARG:O	1:A:49:GLU:HG2	2.18	0.43
1:A:99:GLN:HB3	1:A:101:HIS:ND1	2.33	0.43
1:D:166:GLN:CD	1:D:168:ARG:HH22	2.26	0.43
1:D:178:ARG:NH1	1:D:181:LYS:HD2	2.34	0.43
1:D:231:ALA:CA	1:D:234:MET:HE2	2.48	0.43
1:E:58:ASP:OD2	1:E:250:ARG:HD3	2.18	0.43
1:E:76:ILE:HG22	1:E:80:GLU:HG3	1.99	0.43
1:A:34:ILE:CA	1:A:37:LEU:HD23	2.49	0.43
1:A:160:ASP:O	1:F:72:PRO:HB3	2.18	0.43
1:B:77:ALA:O	1:B:81:LEU:HG	2.19	0.43
1:B:94:THR:OG1	2:B:254:ACY:O	2.32	0.43
1:F:97:ALA:HB1	1:F:102:ILE:HB	2.01	0.43
1:F:113:SER:HA	1:F:155:VAL:HG13	2.01	0.43
1:A:175:ARG:NH1	1:A:175:ARG:HG2	2.34	0.43
1:D:102:ILE:HD13	1:D:108:LEU:HD21	2.00	0.43
1:E:161:THR:HB	1:E:165:GLY:CA	2.48	0.43
1:F:8:HIS:HB2	1:F:80:GLU:CD	2.43	0.43
1:F:220:ILE:HG13	1:F:221:VAL:H	1.81	0.43
1:B:146:SER:O	1:B:147:ILE:HG13	2.18	0.43
1:C:115:ARG:NH2	1:C:121:LEU:HD23	2.34	0.43
1:F:57:LEU:HB3	1:F:253:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:THR:OG1	1:F:194:ASN:ND2	2.47	0.43
1:C:6:VAL:HG21	1:C:10:GLY:N	2.34	0.43
1:C:173:SER:HB3	1:E:209:GLN:HE21	1.84	0.43
1:D:168:ARG:HG3	1:D:223:ARG:HH12	1.84	0.43
1:A:169:TYR:O	1:A:171:THR:N	2.51	0.43
1:B:76:ILE:HD11	1:D:162:PHE:CE2	2.54	0.43
1:B:126:MET:CE	1:F:127:GLU:HA	2.47	0.43
1:C:12:THR:O	1:C:15:ASP:HB2	2.19	0.43
1:C:35:ALA:O	1:C:41:PRO:HB3	2.19	0.43
1:C:237:THR:O	1:C:242:VAL:HG23	2.19	0.43
1:D:102:ILE:HG12	1:D:152:HIS:NE2	2.34	0.43
1:D:147:ILE:HD11	1:D:149:ALA:CB	2.36	0.43
1:F:147:ILE:O	1:F:147:ILE:HG13	2.18	0.43
1:B:16:LEU:N	1:B:16:LEU:HD22	2.34	0.43
1:C:25:PRO:C	1:C:67:THR:HG23	2.44	0.43
1:D:151:THR:CG2	1:D:152:HIS:H	2.32	0.43
1:E:8:HIS:ND1	1:E:8:HIS:N	2.66	0.43
1:E:39:ASP:HA	1:F:145:LYS:CE	2.49	0.43
1:E:40:LYS:H	1:E:41:PRO:CD	2.32	0.43
1:E:165:GLY:O	1:E:166:GLN:C	2.60	0.43
1:E:167:GLU:HB2	1:E:183:SER:OG	2.18	0.43
1:F:34:ILE:O	1:F:35:ALA:C	2.61	0.43
1:F:163:TYR:N	1:F:164:PRO:CD	2.82	0.43
1:D:230:ASN:ND2	1:D:233:THR:OG1	2.52	0.42
1:E:92:ILE:CD1	1:E:93:GLY:H	2.32	0.42
1:F:34:ILE:HD13	1:F:242:VAL:HG22	2.01	0.42
1:A:30:ARG:HG2	1:A:30:ARG:NH1	2.34	0.42
1:A:106:ASP:HB2	1:A:219:VAL:CG2	2.48	0.42
1:C:172:TYR:HB2	1:E:83:GLN:CG	2.49	0.42
1:C:223:ARG:C	1:C:225:GLN:N	2.76	0.42
1:C:229:PRO:HG2	1:C:230:ASN:H	1.83	0.42
1:D:20:GLN:HA	1:D:86:ILE:HA	2.00	0.42
1:D:92:ILE:CD1	1:D:242:VAL:HA	2.49	0.42
1:E:23:ILE:HA	1:E:90:LEU:O	2.19	0.42
1:E:76:ILE:O	1:E:80:GLU:CG	2.67	0.42
1:E:141:VAL:O	1:E:145:LYS:N	2.51	0.42
1:A:221:VAL:O	1:A:221:VAL:CG1	2.65	0.42
1:B:128:PHE:CD1	1:B:129:PRO:CD	3.02	0.42
1:B:203:LEU:O	1:B:204:THR:C	2.62	0.42
1:C:81:LEU:HB3	1:C:86:ILE:HD12	2.00	0.42
1:D:163:TYR:HD2	1:D:168:ARG:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:ARG:C	1:E:180:PHE:H	2.26	0.42
1:F:17:GLN:HA	1:F:17:GLN:NE2	2.34	0.42
1:F:49:GLU:C	1:F:50:PHE:CD2	2.96	0.42
1:B:40:LYS:O	1:B:55:ALA:HA	2.19	0.42
1:B:162:PHE:O	1:B:168:ARG:HD2	2.18	0.42
1:C:35:ALA:HA	1:C:38:MET:CE	2.49	0.42
1:C:119:ALA:HB3	1:C:201:THR:OG1	2.18	0.42
1:C:139:ALA:O	1:C:140:LEU:C	2.62	0.42
1:D:144:ALA:HB2	1:D:244:ILE:HD13	2.01	0.42
1:A:79:GLU:OE2	1:F:171:THR:HG21	2.18	0.42
1:B:201:THR:O	1:B:202:LEU:C	2.62	0.42
1:C:22:ALA:CB	1:C:86:ILE:HD13	2.50	0.42
1:D:186:GLU:O	1:D:190:MET:HG3	2.19	0.42
1:B:40:LYS:NZ	1:C:43:LYS:HD2	2.35	0.42
1:D:166:GLN:HG2	1:D:195:TYR:CE1	2.54	0.42
1:E:52:SER:HB3	1:E:65:CYS:SG	2.58	0.42
1:F:12:THR:O	1:F:13:LYS:C	2.62	0.42
1:F:166:GLN:O	1:F:167:GLU:C	2.61	0.42
1:A:99:GLN:HA	1:A:100:PRO:HD3	1.78	0.42
1:A:160:ASP:HB3	1:F:119:ALA:CB	2.49	0.42
1:B:40:LYS:HZ1	1:C:43:LYS:HD2	1.84	0.42
1:B:142:GLU:O	1:B:143:ALA:C	2.63	0.42
1:C:172:TYR:CD2	1:C:172:TYR:C	2.97	0.42
1:D:34:ILE:HG22	1:D:38:MET:CE	2.49	0.42
1:D:236:GLN:O	1:D:237:THR:C	2.63	0.42
1:E:57:LEU:HD11	1:E:250:ARG:NE	2.35	0.42
1:E:184:MET:HE3	1:E:188:GLN:HE22	1.84	0.42
1:F:7:PHE:O	1:F:7:PHE:CD1	2.72	0.42
1:F:71:GLY:O	1:F:75:SER:OG	2.31	0.42
1:F:90:LEU:HD11	1:F:252:LEU:HD12	2.02	0.42
1:F:187:TRP:HB3	1:F:192:VAL:CG2	2.41	0.42
1:A:9:LEU:HD12	1:A:80:GLU:HB3	2.02	0.42
1:B:57:LEU:HD21	1:B:250:ARG:CG	2.49	0.42
1:C:80:GLU:O	1:C:83:GLN:HB2	2.19	0.42
1:E:70:GLY:O	1:E:73:SER:HB3	2.20	0.42
1:F:117:ASP:OD1	1:F:120:SER:OG	2.34	0.42
1:F:147:ILE:CD1	1:F:244:ILE:HD11	2.45	0.42
1:B:15:ASP:HB3	1:B:44:LEU:CD2	2.49	0.42
1:C:163:TYR:CD1	1:E:79:GLU:OE1	2.72	0.42
1:C:236:GLN:O	1:C:240:HIS:HB2	2.18	0.42
1:A:108:LEU:O	1:A:216:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:THR:HG21	1:D:220:ILE:HG23	2.02	0.42
1:E:196:GLU:OE2	1:E:199:SER:N	2.52	0.42
1:F:108:LEU:HA	1:F:152:HIS:O	2.20	0.42
1:F:174:GLY:O	1:F:175:ARG:HB3	2.19	0.42
1:F:194:ASN:H	1:F:194:ASN:ND2	2.00	0.42
1:A:50:PHE:CE2	1:A:77:ALA:HB2	2.55	0.41
1:A:226:GLN:HE21	1:A:226:GLN:HB3	1.59	0.41
1:C:98:ILE:O	1:C:224:THR:CG2	2.68	0.41
1:C:143:ALA:HA	1:C:247:GLU:OE2	2.19	0.41
1:D:12:THR:C	1:D:14:ASN:N	2.77	0.41
1:F:22:ALA:HB2	1:F:86:ILE:CD1	2.45	0.41
1:F:163:TYR:HA	1:F:168:ARG:HB2	2.02	0.41
1:B:78:VAL:HG21	1:B:205:MET:HE3	2.01	0.41
1:B:126:MET:C	1:F:126:MET:HE1	2.44	0.41
1:C:41:PRO:O	1:C:42:VAL:HG22	2.20	0.41
1:F:6:VAL:HG23	1:F:10:GLY:H	1.84	0.41
1:F:98:ILE:HG23	1:F:184:MET:HG3	2.02	0.41
1:A:49:GLU:OE2	1:F:48:ARG:O	2.38	0.41
1:B:40:LYS:HD2	1:B:56:GLU:HB2	2.01	0.41
1:C:147:ILE:CD1	1:C:244:ILE:HG12	2.50	0.41
1:F:233:THR:C	1:F:235:LYS:N	2.77	0.41
1:A:163:TYR:O	1:A:168:ARG:HB2	2.20	0.41
1:B:60:LYS:HB3	1:B:253:LEU:HD22	2.03	0.41
1:D:81:LEU:C	1:D:83:GLN:N	2.78	0.41
1:D:141:VAL:O	1:D:141:VAL:HG12	2.20	0.41
1:B:216:VAL:HG22	1:B:217:ALA:N	2.35	0.41
1:C:48:ARG:HB3	1:C:49:GLU:H	1.52	0.41
1:C:49:GLU:CG	1:E:49:GLU:OE2	2.67	0.41
1:C:232:GLU:OE2	1:C:235:LYS:HB3	2.21	0.41
1:E:232:GLU:O	1:E:236:GLN:HG3	2.20	0.41
1:F:161:THR:OG1	1:F:165:GLY:HA3	2.21	0.41
1:A:169:TYR:CE2	1:A:176:VAL:HG23	2.56	0.41
1:B:151:THR:C	1:B:152:HIS:HD2	2.28	0.41
1:D:176:VAL:O	1:D:177:VAL:O	2.38	0.41
1:E:28:PRO:HA	1:E:31:VAL:CG2	2.49	0.41
1:F:179:ARG:HE	1:F:179:ARG:HB2	1.50	0.41
1:A:7:PHE:O	1:A:9:LEU:N	2.54	0.41
1:A:240:HIS:C	1:A:242:VAL:N	2.78	0.41
1:B:33:LYS:HE2	1:B:33:LYS:CA	2.32	0.41
1:B:92:ILE:HD12	1:B:93:GLY:H	1.86	0.41
1:C:94:THR:HG22	1:C:220:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:LEU:CD2	1:D:50:PHE:CD1	3.04	0.41
1:D:17:GLN:HE21	1:D:17:GLN:CA	2.17	0.41
1:D:38:MET:HB2	1:D:55:ALA:HB1	2.03	0.41
1:E:16:LEU:HD22	1:E:63:ILE:HD11	2.02	0.41
1:E:57:LEU:HD11	1:E:250:ARG:CG	2.49	0.41
1:E:124:ALA:C	1:E:125:PRO:O	2.64	0.41
1:E:232:GLU:OE2	1:E:235:LYS:HD3	2.21	0.41
1:E:234:MET:O	1:E:238:GLU:HB2	2.21	0.41
1:F:179:ARG:HB3	1:F:180:PHE:HD1	1.86	0.41
1:B:23:ILE:CG2	1:B:24:VAL:N	2.83	0.41
1:D:13:LYS:HA	1:D:84:LEU:HD22	2.02	0.41
1:D:34:ILE:O	1:D:38:MET:HE3	2.21	0.41
1:F:48:ARG:HG2	1:F:48:ARG:NH1	2.36	0.41
1:A:159:SER:O	1:A:197:MET:HG2	2.21	0.41
1:A:163:TYR:CD2	1:A:171:THR:HG22	2.56	0.41
1:A:226:GLN:O	1:A:227:GLU:C	2.63	0.41
1:B:49:GLU:HB2	1:D:49:GLU:HG2	2.03	0.41
1:B:87:ARG:O	1:B:212:ARG:HG3	2.21	0.41
1:B:128:PHE:HD1	1:B:129:PRO:N	2.19	0.41
1:B:184:MET:SD	1:B:223:ARG:HD2	2.61	0.41
1:B:184:MET:HE2	1:B:188:GLN:NE2	2.36	0.41
1:C:16:LEU:O	1:C:17:GLN:C	2.63	0.41
1:C:41:PRO:C	1:C:42:VAL:CG2	2.93	0.41
1:D:38:MET:HB3	1:D:56:GLU:O	2.20	0.41
1:D:126:MET:HE2	1:D:126:MET:HB2	1.91	0.41
1:E:26:GLY:HA2	1:E:67:THR:H	1.86	0.41
1:E:57:LEU:O	1:E:60:LYS:N	2.54	0.41
1:E:70:GLY:C	1:E:72:PRO:HD2	2.46	0.41
1:E:87:ARG:NH1	1:E:87:ARG:CG	2.77	0.41
1:F:11:LEU:HD21	1:F:52:SER:HG	1.84	0.41
1:F:123:PHE:CD1	1:F:123:PHE:N	2.89	0.41
1:A:89:PHE:O	1:A:213:ALA:HA	2.21	0.41
1:A:141:VAL:O	1:A:145:LYS:HG3	2.21	0.41
1:E:11:LEU:HD21	1:E:45:ALA:HB3	2.02	0.41
1:E:218:GLY:O	1:E:220:ILE:HG23	2.21	0.41
1:E:245:VAL:O	1:E:246:VAL:C	2.64	0.41
1:A:90:LEU:HD11	1:A:252:LEU:HD12	2.03	0.40
1:A:227:GLU:O	1:A:227:GLU:HG3	2.21	0.40
1:E:82:ALA:HB2	1:E:89:PHE:HZ	1.87	0.40
1:F:206:CYS:O	1:F:207:ALA:C	2.64	0.40
1:C:40:LYS:HD2	1:C:56:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ILE:HD11	1:C:244:ILE:HD11	2.03	0.40
1:D:112:ALA:HA	1:D:131:VAL:HA	2.03	0.40
1:D:163:TYR:N	1:D:164:PRO:CD	2.82	0.40
1:E:21:LEU:HG	1:E:88:THR:HB	2.03	0.40
1:E:68:GLY:O	1:E:69:ILE:O	2.39	0.40
1:F:91:ARG:HG3	1:F:92:ILE:N	2.36	0.40
1:F:127:GLU:O	1:F:128:PHE:C	2.64	0.40
1:A:34:ILE:C	1:A:36:ALA:N	2.78	0.40
1:A:180:PHE:O	1:A:181:LYS:C	2.64	0.40
1:B:28:PRO:HB3	1:B:49:GLU:O	2.22	0.40
1:B:109:VAL:HG23	1:B:151:THR:CG2	2.52	0.40
1:C:247:GLU:O	1:C:247:GLU:OE1	2.39	0.40
1:C:251:ARG:HG2	1:C:251:ARG:NH1	2.35	0.40
1:D:155:VAL:HG12	1:D:156:THR:N	2.35	0.40
1:F:108:LEU:HD13	1:F:193:MET:CB	2.48	0.40
1:F:183:SER:O	1:F:186:GLU:N	2.55	0.40
1:F:230:ASN:HD21	1:F:232:GLU:H	1.64	0.40
1:A:16:LEU:HD23	1:A:16:LEU:N	2.36	0.40
1:A:180:PHE:O	1:A:183:SER:CB	2.69	0.40
1:B:12:THR:HG23	1:B:15:ASP:OD2	2.21	0.40
1:B:28:PRO:HB2	1:B:51:THR:OG1	2.22	0.40
1:B:48:ARG:HB3	1:B:49:GLU:H	1.60	0.40
1:C:6:VAL:HB	1:C:80:GLU:OE2	2.21	0.40
1:C:177:VAL:HG13	1:C:179:ARG:HB3	2.04	0.40
1:D:57:LEU:HA	1:D:57:LEU:HD12	1.70	0.40
1:E:8:HIS:CB	1:E:50:PHE:HE1	2.33	0.40
1:E:41:PRO:O	1:E:53:TRP:CZ3	2.75	0.40
1:E:107:VAL:O	1:E:107:VAL:HG23	2.20	0.40
1:E:147:ILE:CD1	1:E:149:ALA:HB2	2.52	0.40
1:F:104:VAL:HG22	1:F:222:ASN:HD22	1.86	0.40
1:A:132:ALA:HB2	1:A:203:LEU:CD2	2.52	0.40
1:A:236:GLN:O	1:A:239:SER:HB2	2.21	0.40
1:A:240:HIS:C	1:A:242:VAL:H	2.28	0.40
1:E:147:ILE:O	1:E:147:ILE:HG12	2.21	0.40
1:E:151:THR:HG22	1:E:152:HIS:N	2.36	0.40
1:E:154:GLY:C	1:E:193:MET:HE2	2.46	0.40
1:F:103:ASN:CB	1:F:106:ASP:OD1	2.69	0.40
1:F:112:ALA:O	1:F:155:VAL:HG13	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	248/253 (98%)	172 (69%)	53 (21%)	23 (9%)	0	1
1	B	248/253 (98%)	174 (70%)	55 (22%)	19 (8%)	1	2
1	C	248/253 (98%)	186 (75%)	40 (16%)	22 (9%)	0	1
1	D	248/253 (98%)	174 (70%)	58 (23%)	16 (6%)	1	3
1	E	248/253 (98%)	166 (67%)	57 (23%)	25 (10%)	0	1
1	F	248/253 (98%)	168 (68%)	59 (24%)	21 (8%)	0	1
All	All	1488/1518 (98%)	1040 (70%)	322 (22%)	126 (8%)	0	1

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	17	GLN
1	A	26	GLY
1	A	167	GLU
1	A	223	ARG
1	A	224	THR
1	A	234	MET
1	B	48	ARG
1	B	167	GLU
1	B	227	GLU
1	B	230	ASN
1	C	6	VAL
1	C	167	GLU
1	C	188	GLN
1	C	230	ASN
1	D	37	LEU
1	D	173	SER
1	D	177	VAL
1	E	5	ASP
1	E	8	HIS

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Mol	Chain	Res	Type
1	E	40	LYS
1	E	69	ILE
1	E	173	SER
1	E	226	GLN
1	E	244	ILE
1	F	35	ALA
1	F	166	GLN
1	F	200	ALA
1	A	177	VAL
1	A	179	ARG
1	A	227	GLU
1	B	13	LYS
1	B	14	ASN
1	B	18	GLY
1	B	170	ASP
1	C	19	ALA
1	C	46	SER
1	C	150	THR
1	C	228	ILE
1	C	229	PRO
1	D	78	VAL
1	D	171	THR
1	D	175	ARG
1	D	189	ALA
1	E	19	ALA
1	E	150	THR
1	E	178	ARG
1	E	181	LYS
1	F	11	LEU
1	F	34	ILE
1	F	58	ASP
1	F	95	THR
1	F	115	ARG
1	F	146	SER
1	F	148	GLY
1	F	172	TYR
1	F	201	THR
1	F	223	ARG
1	A	19	ALA
1	A	49	GLU
1	A	50	PHE
1	A	141	VAL

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Mol	Chain	Res	Type
1	B	85	GLY
1	B	164	PRO
1	B	239	SER
1	C	45	ALA
1	C	118	GLY
1	C	238	GLU
1	D	17	GLN
1	D	146	SER
1	E	27	ASP
1	E	54	ARG
1	E	174	GLY
1	E	221	VAL
1	F	165	GLY
1	F	167	GLU
1	F	186	GLU
1	A	8	HIS
1	A	202	LEU
1	B	178	ARG
1	B	202	LEU
1	B	224	THR
1	C	85	GLY
1	C	138	THR
1	C	170	ASP
1	C	239	SER
1	D	18	GLY
1	D	105	GLY
1	D	147	ILE
1	E	125	PRO
1	E	162	PHE
1	E	179	ARG
1	E	227	GLU
1	E	229	PRO
1	F	15	ASP
1	F	202	LEU
1	A	118	GLY
1	A	170	ASP
1	A	228	ILE
1	B	147	ILE
1	B	203	LEU
1	C	38	MET
1	C	189	ALA
1	C	204	THR

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Mol	Chain	Res	Type
1	D	125	PRO
1	D	223	ARG
1	D	238	GLU
1	E	37	LEU
1	E	48	ARG
1	E	167	GLU
1	F	118	GLY
1	F	244	ILE
1	A	125	PRO
1	B	78	VAL
1	C	40	LYS
1	C	178	ARG
1	B	165	GLY
1	E	85	GLY
1	A	164	PRO
1	E	68	GLY
1	A	25	PRO
1	F	177	VAL
1	A	40	LYS
1	C	164	PRO
1	D	104	VAL
1	B	219	VAL

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	199/202 (98%)	176 (88%)	23 (12%)	5	18
1	B	199/202 (98%)	183 (92%)	16 (8%)	11	34
1	C	199/202 (98%)	180 (90%)	19 (10%)	8	26
1	D	199/202 (98%)	168 (84%)	31 (16%)	2	9
1	E	199/202 (98%)	176 (88%)	23 (12%)	5	18
1	F	199/202 (98%)	171 (86%)	28 (14%)	3	11
All	All	1194/1212 (98%)	1054 (88%)	140 (12%)	5	17

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	8	HIS
1	A	15	ASP
1	A	16	LEU
1	A	32	GLU
1	A	48	ARG
1	A	54	ARG
1	A	64	VAL
1	A	79	GLU
1	A	81	LEU
1	A	92	ILE
1	A	98	ILE
1	A	138	THR
1	A	147	ILE
1	A	158	SER
1	A	160	ASP
1	A	166	GLN
1	A	179	ARG
1	A	196	GLU
1	A	216	VAL
1	A	224	THR
1	A	226	GLN
1	A	228	ILE
1	B	5	ASP
1	B	12	THR
1	B	16	LEU
1	B	17	GLN
1	B	37	LEU
1	B	42	VAL
1	B	47	HIS
1	B	69	ILE
1	B	92	ILE
1	B	94	THR
1	B	160	ASP
1	B	167	GLU
1	B	194	ASN
1	B	196	GLU
1	B	215	MET
1	B	228	ILE
1	C	14	ASN
1	C	32	GLU
1	C	48	ARG

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Mol	Chain	Res	Type
1	C	54	ARG
1	C	62	VAL
1	C	79	GLU
1	C	92	ILE
1	C	98	ILE
1	C	104	VAL
1	C	108	LEU
1	C	147	ILE
1	C	187	TRP
1	C	192	VAL
1	C	196	GLU
1	C	206	CYS
1	C	220	ILE
1	C	230	ASN
1	C	240	HIS
1	C	247	GLU
1	D	12	THR
1	D	15	ASP
1	D	16	LEU
1	D	21	LEU
1	D	29	GLU
1	D	43	LYS
1	D	57	LEU
1	D	58	ASP
1	D	78	VAL
1	D	83	GLN
1	D	86	ILE
1	D	92	ILE
1	D	94	THR
1	D	95	THR
1	D	126	MET
1	D	167	GLU
1	D	170	ASP
1	D	177	VAL
1	D	178	ARG
1	D	179	ARG
1	D	185	GLU
1	D	194	ASN
1	D	195	TYR
1	D	196	GLU
1	D	219	VAL
1	D	224	THR

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Mol	Chain	Res	Type
1	D	225	GLN
1	D	228	ILE
1	D	234	MET
1	D	238	GLU
1	D	239	SER
1	E	16	LEU
1	E	17	GLN
1	E	37	LEU
1	E	44	LEU
1	E	47	HIS
1	E	54	ARG
1	E	69	ILE
1	E	92	ILE
1	E	126	MET
1	E	147	ILE
1	E	153	VAL
1	E	160	ASP
1	E	161	THR
1	E	167	GLU
1	E	171	THR
1	E	180	PHE
1	E	194	ASN
1	E	195	TYR
1	E	196	GLU
1	E	215	MET
1	E	227	GLU
1	E	228	ILE
1	E	238	GLU
1	F	11	LEU
1	F	12	THR
1	F	17	GLN
1	F	38	MET
1	F	48	ARG
1	F	50	PHE
1	F	54	ARG
1	F	98	ILE
1	F	104	VAL
1	F	106	ASP
1	F	107	VAL
1	F	108	LEU
1	F	110	THR
1	F	126	MET

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Mol	Chain	Res	Type
1	F	138	THR
1	F	151	THR
1	F	172	TYR
1	F	179	ARG
1	F	185	GLU
1	F	194	ASN
1	F	196	GLU
1	F	205	MET
1	F	206	CYS
1	F	209	GLN
1	F	215	MET
1	F	219	VAL
1	F	234	MET
1	F	239	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	20	GLN
1	A	83	GLN
1	A	209	GLN
1	A	225	GLN
1	A	226	GLN
1	A	230	ASN
1	A	236	GLN
1	B	14	ASN
1	B	17	GLN
1	B	103	ASN
1	B	152	HIS
1	B	166	GLN
1	B	188	GLN
1	B	194	ASN
1	B	209	GLN
1	C	14	ASN
1	C	17	GLN
1	C	83	GLN
1	C	188	GLN
1	C	194	ASN
1	C	225	GLN
1	C	236	GLN
1	D	17	GLN

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Mol	Chain	Res	Type
1	D	166	GLN
1	D	194	ASN
1	D	209	GLN
1	D	222	ASN
1	D	225	GLN
1	D	226	GLN
1	D	230	ASN
1	E	17	GLN
1	E	47	HIS
1	E	83	GLN
1	E	194	ASN
1	E	209	GLN
1	E	222	ASN
1	E	240	HIS
1	F	17	GLN
1	F	83	GLN
1	F	166	GLN
1	F	194	ASN
1	F	209	GLN
1	F	222	ASN
1	F	230	ASN

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	ACY	B	255	-	3,3,3	1.65	0	3,3,3	1.29	0
2	ACY	B	254	-	3,3,3	1.49	0	3,3,3	1.37	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	254	ACY	5	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.