



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:25 PM UTC

PDB ID : 1OEL / pdb_00001oel
Title : CONFORMATIONAL VARIABILITY IN THE REFINED STRUCTURE OF
THE CHAPERONIN GROEL AT 2.8 ANGSTROM RESOLUTION
Authors : Braig, K.; Adams, P.D.; Brunger, A.T.
Deposited on : 1995-11-21
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **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

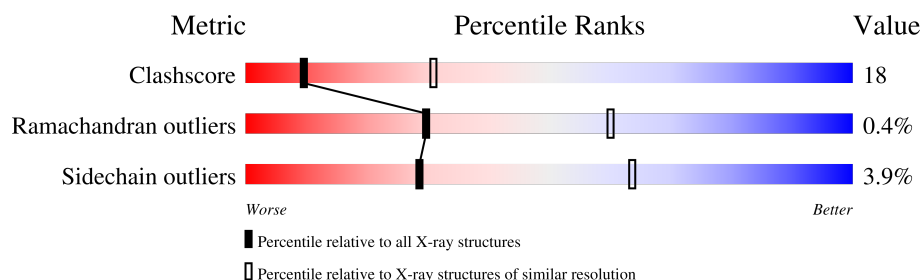
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	547	63% 31% . .
1	B	547	62% 32% . .
1	C	547	63% 31% . .
1	D	547	62% 32% . .
1	E	547	63% 31% . .
1	F	547	63% 30% . .
1	G	547	63% 31% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27078 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 GROEL (HSP60 CLASS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	B	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	C	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	D	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	E	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	F	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	G	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	engineered mutation	UNP P0A6F5
A	126	VAL	ALA	engineered mutation	UNP P0A6F5
B	13	GLY	ARG	engineered mutation	UNP P0A6F5
B	126	VAL	ALA	engineered mutation	UNP P0A6F5
C	13	GLY	ARG	engineered mutation	UNP P0A6F5
C	126	VAL	ALA	engineered mutation	UNP P0A6F5
D	13	GLY	ARG	engineered mutation	UNP P0A6F5
D	126	VAL	ALA	engineered mutation	UNP P0A6F5
E	13	GLY	ARG	engineered mutation	UNP P0A6F5
E	126	VAL	ALA	engineered mutation	UNP P0A6F5
F	13	GLY	ARG	engineered mutation	UNP P0A6F5
F	126	VAL	ALA	engineered mutation	UNP P0A6F5
G	13	GLY	ARG	engineered mutation	UNP P0A6F5
G	126	VAL	ALA	engineered mutation	UNP P0A6F5

- Molecule 2 is water.

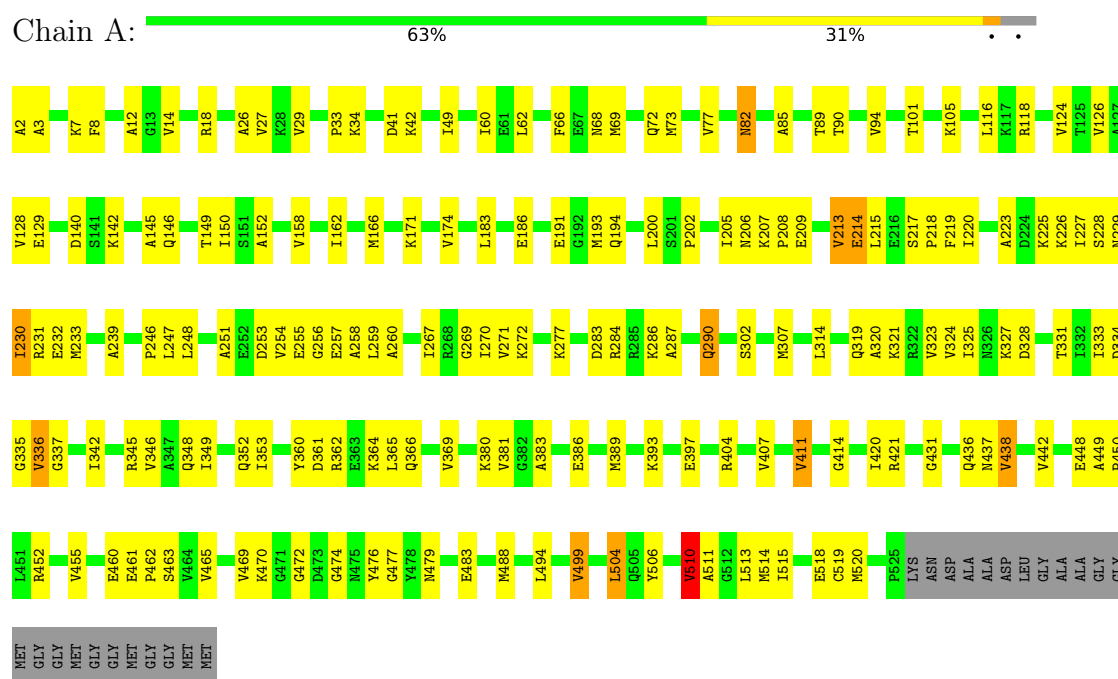
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total 18	O 18	0	0
2	B	23	Total 23	O 23	0	0
2	C	17	Total 17	O 17	0	0
2	D	18	Total 18	O 18	0	0
2	E	36	Total 36	O 36	0	0
2	F	18	Total 18	O 18	0	0
2	G	19	Total 19	O 19	0	0

3 Residue-property plots

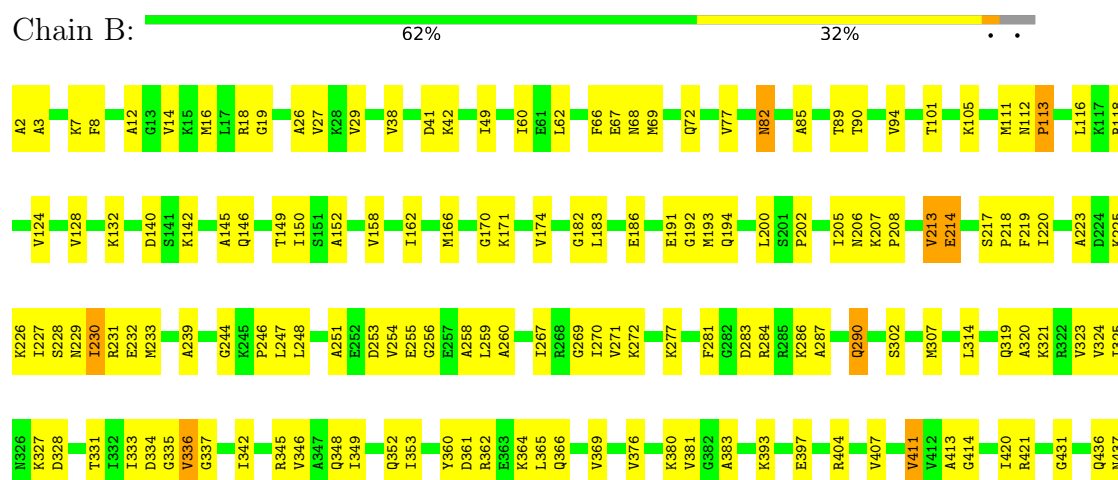
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

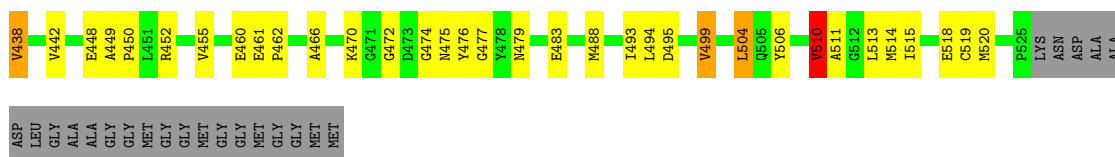
Note EDS was not executed.

• Molecule 1: GROEL (HSP60 CLASS)



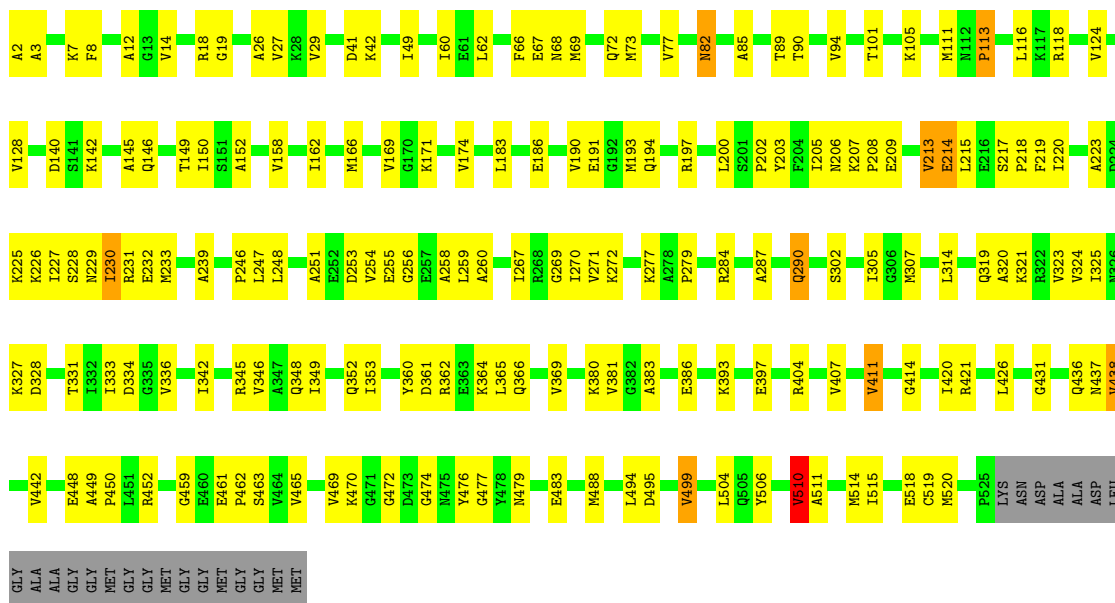
• Molecule 1: GROEL (HSP60 CLASS)





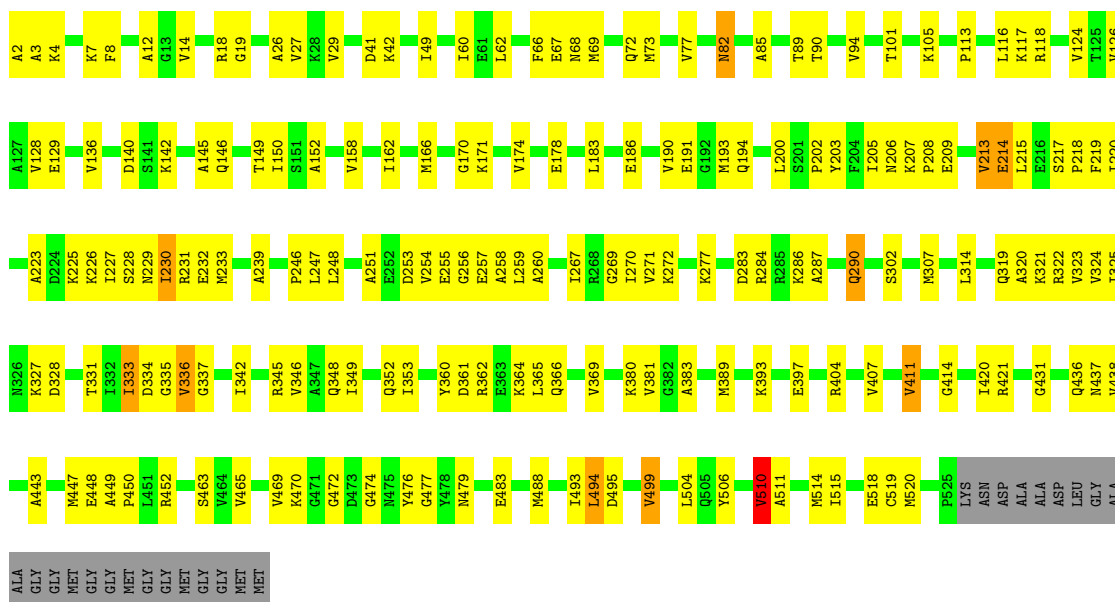
• Molecule 1: GROEL (HSP60 CLASS)

Chain C: 63% 31%

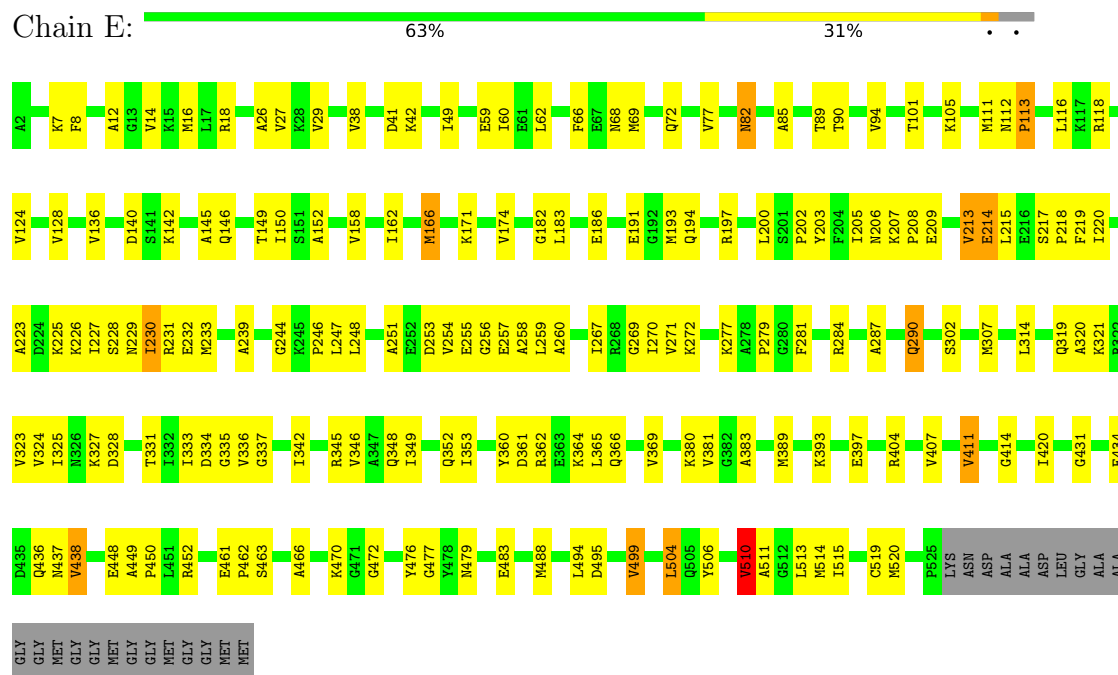


• Molecule 1: GROEL (HSP60 CLASS)

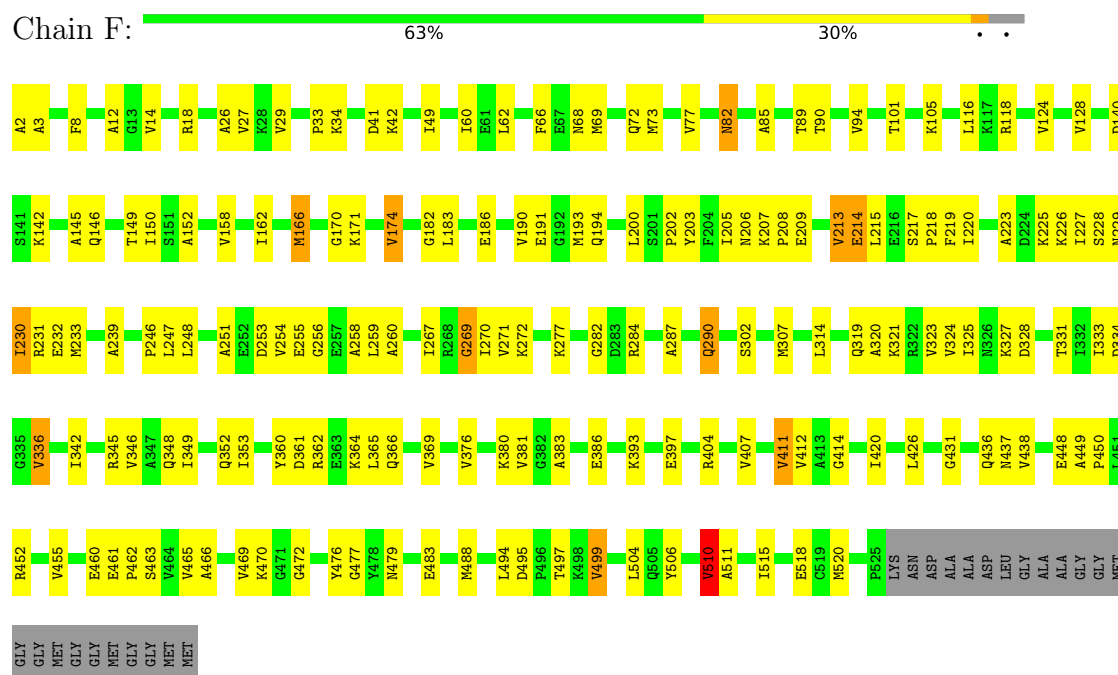
Chain D: 62% 32%



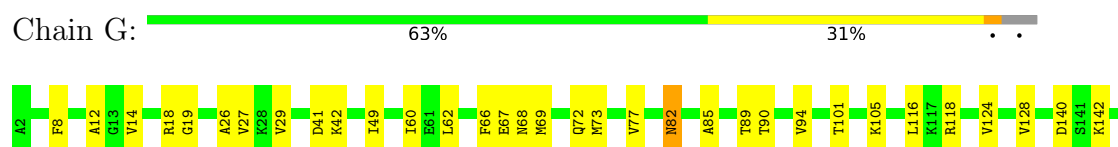
• Molecule 1: GROEL (HSP60 CLASS)



• Molecule 1: GROEL (HSP60 CLASS)



• Molecule 1: GROEL (HSP60 CLASS)



MET	S463	D394	R231	A145
	V464	G335	E232	Q146
	V465	V336	M233	
	A466	G337		T149
MET	V469	I342	A239	I150
	K470			S151
	G471	R345	P246	A152
	G472	V346	L247	
	D473	A347	L248	V158
	G474	Q348		
	M475	I349	A251	I162
	V476		E252	M166
	V477	Q352	D253	
	V478	I353	V254	V169
	M479		E255	G170
		V360	G256	K171
	E483	D361	E957	
		R362	A258	V174
	M488	E363	L259	
		K364	A260	T181
	L493	L365	I267	G182
	L494	Q366	R968	L183
			G269	
	V499	V369	I270	E186
	L504	K380	V271	
	G505	V381	K272	V190
	Y506	G382		E191
	V510	A383	K277	G192
	A511			M193
	G512	M389	F281	Q194
	L513	K393	G282	L200
	M514		R284	S201
	I515	E397	R985	P202
			K286	Y203
	E518	R404	A287	F204
	C519	V407		I205
	M520		Q290	N206
				K207
		V411	S302	P208
	F525	G414	M307	E209
	LYS			V213
	ASN		L314	E214
	ASP	I420		L215
	ALA	R421	Q319	F216
	ASP		A320	S217
	LEU	G431	R321	P218
	GLY	Q436	R322	F219
	ALA	V437	V323	I220
	ALA	N437	I324	
	GLY	V438	I325	A223
			R326	D224
	GLY	E448	K327	K225
	GLY	M449	D328	K226
	MET	P450		I227
	GLY	L451	T331	S228
	GLY	R452	I332	N229
		I322	T230	

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	178.38Å 204.98Å 280.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	72.2 (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.227 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27078	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0/3875	0.86	3/5234 (0.1%)
1	B	0.55	0/3875	0.85	3/5234 (0.1%)
1	C	0.53	0/3875	0.85	3/5234 (0.1%)
1	D	0.53	0/3875	0.85	3/5234 (0.1%)
1	E	0.56	0/3875	0.86	5/5234 (0.1%)
1	F	0.51	0/3875	0.85	3/5234 (0.1%)
1	G	0.52	0/3875	0.85	3/5234 (0.1%)
All	All	0.53	0/27125	0.85	23/36638 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	333	ILE	N-CA-C	7.66	118.46	110.72
1	C	333	ILE	N-CA-C	7.60	118.39	110.72
1	G	333	ILE	N-CA-C	7.59	118.39	110.72
1	F	333	ILE	N-CA-C	7.58	118.38	110.72
1	D	333	ILE	N-CA-C	7.46	118.25	110.72
1	B	333	ILE	N-CA-C	7.45	118.25	110.72
1	A	333	ILE	N-CA-C	7.29	118.08	110.72
1	E	112	ASN	CA-C-N	6.19	125.68	119.24
1	E	112	ASN	C-N-CA	6.19	125.68	119.24
1	A	510	VAL	CB-CA-C	-5.75	104.38	112.14
1	E	510	VAL	CB-CA-C	-5.63	104.53	112.14
1	C	60	ILE	N-CA-C	5.54	116.34	107.98
1	G	60	ILE	N-CA-C	5.53	116.33	107.98
1	F	510	VAL	CB-CA-C	-5.53	104.68	112.14
1	B	60	ILE	N-CA-C	5.46	116.23	107.98
1	D	60	ILE	N-CA-C	5.45	116.20	107.98
1	F	60	ILE	N-CA-C	5.42	116.16	107.98
1	G	510	VAL	CB-CA-C	-5.37	104.89	112.14
1	C	510	VAL	CB-CA-C	-5.35	104.92	112.14
1	E	60	ILE	N-CA-C	5.34	116.05	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	510	VAL	CB-CA-C	-5.34	104.93	112.14
1	A	60	ILE	N-CA-C	5.33	116.03	107.98
1	B	510	VAL	CB-CA-C	-5.24	105.06	112.14

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	3847	0	3966	144	0
1	B	3847	0	3966	148	0
1	C	3847	0	3966	142	0
1	D	3847	0	3966	151	0
1	E	3847	0	3966	143	0
1	F	3847	0	3966	143	0
1	G	3847	0	3966	144	0
2	A	18	0	0	0	0
2	B	23	0	0	0	0
2	C	17	0	0	0	0
2	D	18	0	0	1	0
2	E	36	0	0	0	0
2	F	18	0	0	0	0
2	G	19	0	0	0	0
All	All	27078	0	27762	975	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 18.

All (975) 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:E:166:MET:HG2	1:E:171:LYS:HA	1.58	0.86
1:F:166:MET:HG2	1:F:171:LYS:HA	1.59	0.85
1:A:166:MET:HG2	1:A:171:LYS:HA	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:MET:HG2	1:D:171:LYS:HA	1.61	0.83
1:G:166:MET:HG2	1:G:171:LYS:HA	1.60	0.83
1:C:166:MET:HG2	1:C:171:LYS:HA	1.60	0.83
1:C:229:ASN:HA	1:C:258:ALA:HB3	1.61	0.83
1:B:166:MET:HG2	1:B:171:LYS:HA	1.60	0.82
1:B:229:ASN:HA	1:B:258:ALA:HB3	1.62	0.80
1:D:229:ASN:HA	1:D:258:ALA:HB3	1.62	0.80
1:F:229:ASN:HA	1:F:258:ALA:HB3	1.60	0.80
1:A:229:ASN:HA	1:A:258:ALA:HB3	1.61	0.80
1:D:327:LYS:H	1:D:327:LYS:HD2	1.47	0.79
1:E:229:ASN:HA	1:E:258:ALA:HB3	1.62	0.79
1:G:229:ASN:HA	1:G:258:ALA:HB3	1.62	0.79
1:F:327:LYS:H	1:F:327:LYS:HD2	1.48	0.79
1:E:327:LYS:H	1:E:327:LYS:HD2	1.47	0.78
1:B:327:LYS:H	1:B:327:LYS:HD2	1.48	0.78
1:G:327:LYS:H	1:G:327:LYS:HD2	1.48	0.78
1:A:254:VAL:HG13	1:A:259:LEU:HD23	1.66	0.77
1:E:431:GLY:H	1:E:437:ASN:HD21	1.30	0.77
1:E:254:VAL:HG13	1:E:259:LEU:HD23	1.67	0.77
1:F:284:ARG:NH2	1:G:182:GLY:HA2	2.00	0.77
1:C:327:LYS:H	1:C:327:LYS:HD2	1.49	0.77
1:A:68:ASN:O	1:A:72:GLN:HG2	1.84	0.76
1:A:327:LYS:H	1:A:327:LYS:HD2	1.49	0.76
1:D:254:VAL:HG13	1:D:259:LEU:HD23	1.67	0.76
1:B:254:VAL:HG13	1:B:259:LEU:HD23	1.66	0.75
1:G:68:ASN:O	1:G:72:GLN:HG2	1.85	0.75
1:F:254:VAL:HG13	1:F:259:LEU:HD23	1.66	0.75
1:B:431:GLY:H	1:B:437:ASN:HD21	1.32	0.75
1:C:68:ASN:O	1:C:72:GLN:HG2	1.85	0.74
1:C:254:VAL:HG13	1:C:259:LEU:HD23	1.68	0.74
1:G:254:VAL:HG13	1:G:259:LEU:HD23	1.67	0.74
1:B:68:ASN:O	1:B:72:GLN:HG2	1.86	0.74
1:F:68:ASN:O	1:F:72:GLN:HG2	1.86	0.73
1:A:431:GLY:H	1:A:437:ASN:HD21	1.33	0.73
1:D:431:GLY:H	1:D:437:ASN:HD21	1.33	0.72
1:G:431:GLY:H	1:G:437:ASN:HD21	1.33	0.72
1:E:68:ASN:O	1:E:72:GLN:HG2	1.89	0.72
1:F:431:GLY:H	1:F:437:ASN:HD21	1.36	0.71
1:C:431:GLY:H	1:C:437:ASN:HD21	1.37	0.70
1:D:230:ILE:HG23	1:D:259:LEU:HA	1.73	0.70
1:E:431:GLY:H	1:E:437:ASN:ND2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ILE:HG23	1:C:259:LEU:HA	1.73	0.70
1:F:230:ILE:HG23	1:F:259:LEU:HA	1.73	0.70
1:G:230:ILE:HG23	1:G:259:LEU:HA	1.73	0.69
1:D:431:GLY:H	1:D:437:ASN:ND2	1.90	0.69
1:E:230:ILE:HG23	1:E:259:LEU:HA	1.73	0.69
1:A:230:ILE:HG23	1:A:259:LEU:HA	1.73	0.69
1:D:68:ASN:O	1:D:72:GLN:HG2	1.92	0.69
1:A:62:LEU:H	1:A:68:ASN:HD22	1.40	0.69
1:A:431:GLY:H	1:A:437:ASN:ND2	1.90	0.69
1:B:230:ILE:HG23	1:B:259:LEU:HA	1.73	0.69
1:C:62:LEU:H	1:C:68:ASN:HD22	1.40	0.68
1:E:118:ARG:HD2	1:E:436:GLN:NE2	2.08	0.68
1:F:353:ILE:HG12	1:F:365:LEU:HB3	1.75	0.68
1:B:431:GLY:H	1:B:437:ASN:ND2	1.92	0.68
1:D:227:ILE:HB	1:D:259:LEU:HD22	1.76	0.68
1:A:227:ILE:HB	1:A:259:LEU:HD22	1.76	0.68
1:F:223:ALA:O	1:F:251:ALA:HA	1.94	0.68
1:G:431:GLY:H	1:G:437:ASN:ND2	1.91	0.68
1:F:227:ILE:HB	1:F:259:LEU:HD22	1.76	0.68
1:B:353:ILE:HG12	1:B:365:LEU:HB3	1.75	0.67
1:F:62:LEU:H	1:F:68:ASN:HD22	1.41	0.67
1:E:227:ILE:HB	1:E:259:LEU:HD22	1.77	0.67
1:G:223:ALA:O	1:G:251:ALA:HA	1.94	0.67
1:C:223:ALA:O	1:C:251:ALA:HA	1.95	0.67
1:D:353:ILE:HG12	1:D:365:LEU:HB3	1.75	0.67
1:D:223:ALA:O	1:D:251:ALA:HA	1.95	0.67
1:C:228:SER:HB3	1:C:255:GLU:HB2	1.77	0.67
1:G:227:ILE:HB	1:G:259:LEU:HD22	1.77	0.67
1:A:353:ILE:HG12	1:A:365:LEU:HB3	1.76	0.67
1:B:227:ILE:HB	1:B:259:LEU:HD22	1.76	0.67
1:E:302:SER:H	1:E:307:MET:HG3	1.60	0.67
1:E:353:ILE:HG12	1:E:365:LEU:HB3	1.76	0.67
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.77	0.67
1:G:420:ILE:HG13	1:G:448:GLU:HG2	1.77	0.67
1:A:228:SER:HB3	1:A:255:GLU:HB2	1.78	0.66
1:F:431:GLY:H	1:F:437:ASN:ND2	1.93	0.66
1:C:227:ILE:HB	1:C:259:LEU:HD22	1.77	0.66
1:B:223:ALA:O	1:B:251:ALA:HA	1.95	0.66
1:E:223:ALA:O	1:E:251:ALA:HA	1.95	0.66
1:D:228:SER:HB3	1:D:255:GLU:HB2	1.77	0.66
1:F:420:ILE:HG13	1:F:448:GLU:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:O	1:A:251:ALA:HA	1.95	0.66
1:C:353:ILE:HG12	1:C:365:LEU:HB3	1.77	0.66
1:D:302:SER:H	1:D:307:MET:HG3	1.61	0.66
1:E:228:SER:HB3	1:E:255:GLU:HB2	1.78	0.66
1:G:228:SER:HB3	1:G:255:GLU:HB2	1.78	0.66
1:B:62:LEU:H	1:B:68:ASN:HD22	1.41	0.66
1:C:14:VAL:O	1:C:18:ARG:HG3	1.94	0.66
1:F:233:MET:SD	1:F:259:LEU:HD11	2.36	0.66
1:F:228:SER:HB3	1:F:255:GLU:HB2	1.78	0.65
1:G:118:ARG:HD2	1:G:436:GLN:NE2	2.12	0.65
1:G:353:ILE:HG12	1:G:365:LEU:HB3	1.78	0.65
1:B:228:SER:HB3	1:B:255:GLU:HB2	1.79	0.65
1:G:302:SER:H	1:G:307:MET:HG3	1.60	0.65
1:D:62:LEU:H	1:D:68:ASN:HD22	1.41	0.65
1:B:302:SER:H	1:B:307:MET:HG3	1.60	0.65
1:D:118:ARG:HD2	1:D:436:GLN:NE2	2.12	0.65
1:C:233:MET:SD	1:C:259:LEU:HD11	2.37	0.65
1:F:302:SER:H	1:F:307:MET:HG3	1.61	0.65
1:B:14:VAL:O	1:B:18:ARG:HG3	1.96	0.65
1:C:302:SER:H	1:C:307:MET:HG3	1.60	0.65
1:F:118:ARG:HD2	1:F:436:GLN:NE2	2.12	0.65
1:G:202:PRO:O	1:G:205:ILE:HG12	1.97	0.65
1:A:202:PRO:O	1:A:205:ILE:HG12	1.97	0.65
1:D:145:ALA:O	1:D:149:THR:HG23	1.97	0.64
1:G:145:ALA:O	1:G:149:THR:HG23	1.97	0.64
1:A:302:SER:H	1:A:307:MET:HG3	1.62	0.64
1:C:431:GLY:H	1:C:437:ASN:ND2	1.95	0.64
1:D:14:VAL:O	1:D:18:ARG:HG3	1.96	0.64
1:E:145:ALA:O	1:E:149:THR:HG23	1.97	0.64
1:E:281:PHE:HB3	1:F:386:GLU:OE1	1.98	0.64
1:G:14:VAL:O	1:G:18:ARG:HG3	1.97	0.64
1:A:233:MET:SD	1:A:259:LEU:HD11	2.38	0.64
1:B:202:PRO:O	1:B:205:ILE:HG12	1.98	0.64
1:G:62:LEU:H	1:G:68:ASN:HD22	1.42	0.64
1:C:62:LEU:H	1:C:68:ASN:ND2	1.95	0.64
1:A:14:VAL:O	1:A:18:ARG:HG3	1.98	0.63
1:B:248:LEU:HD22	1:B:323:VAL:HG11	1.78	0.63
1:C:118:ARG:HD2	1:C:436:GLN:NE2	2.13	0.63
1:D:233:MET:SD	1:D:259:LEU:HD11	2.37	0.63
1:E:62:LEU:H	1:E:68:ASN:HD22	1.44	0.63
1:B:145:ALA:O	1:B:149:THR:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:PRO:O	1:C:205:ILE:HG12	1.98	0.63
1:F:202:PRO:O	1:F:205:ILE:HG12	1.98	0.63
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.81	0.63
1:G:248:LEU:HD22	1:G:323:VAL:HG11	1.81	0.63
1:A:118:ARG:HD2	1:A:436:GLN:NE2	2.14	0.63
1:A:62:LEU:H	1:A:68:ASN:ND2	1.97	0.63
1:E:62:LEU:H	1:E:68:ASN:ND2	1.97	0.63
1:F:248:LEU:HD22	1:F:323:VAL:HG11	1.81	0.63
1:B:62:LEU:H	1:B:68:ASN:ND2	1.97	0.63
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.81	0.63
1:E:420:ILE:HG13	1:E:448:GLU:HG2	1.80	0.63
1:A:68:ASN:ND2	1:A:72:GLN:HE21	1.96	0.62
1:D:62:LEU:H	1:D:68:ASN:ND2	1.97	0.62
1:A:145:ALA:O	1:A:149:THR:HG23	1.98	0.62
1:B:233:MET:SD	1:B:259:LEU:HD11	2.39	0.62
1:G:62:LEU:H	1:G:68:ASN:ND2	1.97	0.62
1:F:62:LEU:H	1:F:68:ASN:ND2	1.97	0.62
1:C:248:LEU:HD22	1:C:323:VAL:HG11	1.81	0.62
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.82	0.62
1:E:233:MET:SD	1:E:259:LEU:HD11	2.40	0.62
1:E:202:PRO:O	1:E:205:ILE:HG12	1.99	0.62
1:D:257:GLU:OE2	1:E:272:LYS:HE2	2.01	0.61
1:D:420:ILE:HG13	1:D:448:GLU:HG2	1.82	0.61
1:D:202:PRO:O	1:D:205:ILE:HG12	1.99	0.61
1:A:248:LEU:HD22	1:A:323:VAL:HG11	1.82	0.61
1:C:145:ALA:O	1:C:149:THR:HG23	2.01	0.61
1:E:14:VAL:O	1:E:18:ARG:HG3	1.99	0.61
1:A:361:ASP:O	1:A:365:LEU:HD23	2.01	0.61
1:E:248:LEU:HD22	1:E:323:VAL:HG11	1.81	0.61
1:F:14:VAL:O	1:F:18:ARG:HG3	1.99	0.61
1:B:118:ARG:HD2	1:B:436:GLN:NE2	2.16	0.61
1:C:231:ARG:NH2	1:D:270:ILE:O	2.33	0.60
1:D:248:LEU:HD22	1:D:323:VAL:HG11	1.81	0.60
1:E:68:ASN:ND2	1:E:72:GLN:HE21	1.99	0.60
1:F:68:ASN:ND2	1:F:72:GLN:HE21	1.98	0.60
1:A:248:LEU:HD13	1:A:325:ILE:HD11	1.82	0.60
1:F:361:ASP:O	1:F:365:LEU:HD23	2.00	0.60
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.83	0.60
1:A:420:ILE:HG13	1:A:448:GLU:HG2	1.84	0.60
1:B:420:ILE:HG13	1:B:448:GLU:HG2	1.84	0.60
1:B:366:GLN:HA	1:B:369:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ASP:O	1:B:365:LEU:HD23	2.02	0.60
1:E:69:MET:HE3	1:E:520:MET:HE2	1.84	0.60
1:G:361:ASP:O	1:G:365:LEU:HD23	2.01	0.60
1:G:68:ASN:ND2	1:G:72:GLN:HE21	1.99	0.59
1:D:349:ILE:O	1:D:353:ILE:HG13	2.02	0.59
1:D:361:ASP:O	1:D:365:LEU:HD23	2.03	0.59
1:C:361:ASP:O	1:C:365:LEU:HD23	2.01	0.59
1:A:366:GLN:HA	1:A:369:VAL:HG22	1.84	0.59
1:D:248:LEU:HD13	1:D:325:ILE:HD11	1.83	0.59
1:G:233:MET:SD	1:G:259:LEU:HD11	2.42	0.59
1:F:145:ALA:O	1:F:149:THR:HG23	2.02	0.59
1:A:254:VAL:CG1	1:A:259:LEU:HD23	2.32	0.59
1:B:254:VAL:CG1	1:B:259:LEU:HD23	2.32	0.59
1:E:361:ASP:O	1:E:365:LEU:HD23	2.03	0.59
1:C:248:LEU:HD13	1:C:325:ILE:HD11	1.83	0.59
1:G:248:LEU:HD13	1:G:325:ILE:HD11	1.84	0.59
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.85	0.59
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.85	0.58
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.85	0.58
1:B:248:LEU:HD13	1:B:325:ILE:HD11	1.84	0.58
1:F:254:VAL:CG1	1:F:259:LEU:HD23	2.33	0.58
1:E:254:VAL:CG1	1:E:259:LEU:HD23	2.33	0.58
1:A:349:ILE:O	1:A:353:ILE:HG13	2.04	0.58
1:B:349:ILE:O	1:B:353:ILE:HG13	2.03	0.58
1:D:254:VAL:CG1	1:D:259:LEU:HD23	2.34	0.58
1:F:248:LEU:HD13	1:F:325:ILE:HD11	1.83	0.58
1:F:366:GLN:HA	1:F:369:VAL:HG22	1.86	0.58
1:E:366:GLN:HA	1:E:369:VAL:HG22	1.85	0.58
1:F:77:VAL:HG21	1:F:510:VAL:HG13	1.84	0.58
1:C:254:VAL:CG1	1:C:259:LEU:HD23	2.34	0.57
1:D:73:MET:HE3	1:E:49:ILE:CD1	2.33	0.57
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.85	0.57
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.86	0.57
1:D:68:ASN:ND2	1:D:72:GLN:HE21	2.02	0.57
1:A:77:VAL:HG21	1:A:510:VAL:HG13	1.86	0.57
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.85	0.57
1:E:248:LEU:HD13	1:E:325:ILE:HD11	1.85	0.57
1:B:68:ASN:ND2	1:B:72:GLN:HE21	2.03	0.57
1:C:349:ILE:O	1:C:353:ILE:HG13	2.04	0.57
1:E:349:ILE:O	1:E:353:ILE:HG13	2.04	0.57
1:G:349:ILE:O	1:G:353:ILE:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:MET:HE3	1:C:520:MET:HE2	1.86	0.56
1:G:254:VAL:CG1	1:G:259:LEU:HD23	2.34	0.56
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.86	0.56
1:E:513:LEU:HD13	1:F:49:ILE:HD12	1.87	0.56
1:F:349:ILE:O	1:F:353:ILE:HG13	2.04	0.56
1:C:68:ASN:ND2	1:C:72:GLN:HE21	2.03	0.56
1:D:231:ARG:HH22	1:E:244:GLY:HA2	1.71	0.56
1:B:186:GLU:HB2	1:B:380:LYS:HB2	1.87	0.56
1:C:366:GLN:HA	1:C:369:VAL:HG22	1.88	0.56
1:F:284:ARG:HH22	1:G:182:GLY:HA2	1.71	0.56
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.87	0.56
1:C:220:ILE:HD12	1:C:248:LEU:HD23	1.87	0.56
1:F:256:GLY:HA2	1:F:260:ALA:HB3	1.87	0.56
1:G:366:GLN:HA	1:G:369:VAL:HG22	1.88	0.56
1:D:321:LYS:CB	1:D:334:ASP:HB3	2.36	0.56
1:D:366:GLN:HA	1:D:369:VAL:HG22	1.87	0.56
1:F:200:LEU:HD13	1:F:254:VAL:HB	1.88	0.56
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.88	0.56
1:D:73:MET:HE3	1:E:49:ILE:HD11	1.86	0.55
1:F:287:ALA:O	1:F:290:GLN:HB3	2.07	0.55
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.88	0.55
1:F:321:LYS:CB	1:F:334:ASP:HB3	2.36	0.55
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.89	0.55
1:D:284:ARG:NH2	1:E:182:GLY:HA2	2.20	0.55
1:F:69:MET:HE3	1:F:520:MET:HE2	1.88	0.55
1:C:190:VAL:HG22	1:C:191:GLU:N	2.21	0.55
1:C:200:LEU:HD13	1:C:254:VAL:HB	1.89	0.55
1:E:200:LEU:HD13	1:E:254:VAL:HB	1.89	0.55
1:D:77:VAL:HG21	1:D:510:VAL:HG13	1.87	0.55
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.88	0.55
1:F:220:ILE:HD12	1:F:248:LEU:HD23	1.89	0.55
1:C:321:LYS:CB	1:C:334:ASP:HB3	2.37	0.55
1:G:200:LEU:HD13	1:G:254:VAL:HB	1.89	0.55
1:A:231:ARG:HH12	1:B:244:GLY:HA2	1.71	0.55
1:A:321:LYS:CB	1:A:334:ASP:HB3	2.37	0.55
1:B:256:GLY:HA2	1:B:260:ALA:HB3	1.88	0.55
1:C:246:PRO:HB3	1:C:272:LYS:HB2	1.88	0.55
1:D:200:LEU:HD13	1:D:254:VAL:HB	1.89	0.55
1:G:213:VAL:HG13	1:G:325:ILE:HB	1.89	0.55
1:G:511:ALA:O	1:G:515:ILE:HG13	2.06	0.55
1:A:220:ILE:HD12	1:A:248:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:LEU:CD1	1:C:254:VAL:HB	2.37	0.54
1:G:41:ASP:O	1:G:42:LYS:HD3	2.08	0.54
1:G:256:GLY:HA2	1:G:260:ALA:HB3	1.88	0.54
1:B:200:LEU:HD13	1:B:254:VAL:HB	1.89	0.54
1:E:256:GLY:HA2	1:E:260:ALA:HB3	1.88	0.54
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.88	0.54
1:G:220:ILE:HD12	1:G:248:LEU:HD23	1.90	0.54
1:B:321:LYS:CB	1:B:334:ASP:HB3	2.37	0.54
1:C:256:GLY:HA2	1:C:260:ALA:HB3	1.88	0.54
1:B:77:VAL:HG21	1:B:510:VAL:HG13	1.87	0.54
1:D:256:GLY:HA2	1:D:260:ALA:HB3	1.88	0.54
1:B:194:GLN:HE21	1:B:331:THR:HB	1.72	0.54
1:B:220:ILE:HD12	1:B:248:LEU:HD23	1.90	0.54
1:A:194:GLN:HE21	1:A:331:THR:HB	1.73	0.54
1:D:246:PRO:HB3	1:D:272:LYS:HB2	1.90	0.54
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.89	0.54
1:G:321:LYS:CB	1:G:334:ASP:HB3	2.37	0.54
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.88	0.54
1:E:220:ILE:HD12	1:E:248:LEU:HD23	1.89	0.54
1:G:246:PRO:HB3	1:G:272:LYS:HB2	1.89	0.54
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.89	0.54
1:A:246:PRO:HB3	1:A:272:LYS:HB2	1.89	0.54
1:A:342:ILE:O	1:A:346:VAL:HG23	2.08	0.54
1:E:321:LYS:CB	1:E:334:ASP:HB3	2.38	0.54
1:F:219:PHE:O	1:F:247:LEU:HD12	2.08	0.54
1:A:256:GLY:HA2	1:A:260:ALA:HB3	1.89	0.54
1:B:219:PHE:O	1:B:247:LEU:HD12	2.07	0.54
1:F:246:PRO:HB3	1:F:272:LYS:HB2	1.89	0.54
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.89	0.54
1:E:246:PRO:HB3	1:E:272:LYS:HB2	1.90	0.54
1:A:200:LEU:HD13	1:A:254:VAL:HB	1.90	0.53
1:D:287:ALA:O	1:D:290:GLN:HB3	2.07	0.53
1:A:213:VAL:HG13	1:A:325:ILE:HB	1.90	0.53
1:B:200:LEU:CD1	1:B:254:VAL:HB	2.37	0.53
1:E:200:LEU:CD1	1:E:254:VAL:HB	2.38	0.53
1:G:69:MET:HE3	1:G:520:MET:HE2	1.89	0.53
1:G:225:LYS:HG2	1:G:226:LYS:N	2.22	0.53
1:B:124:VAL:O	1:B:128:VAL:HG23	2.09	0.53
1:B:213:VAL:HG13	1:B:325:ILE:HB	1.91	0.53
1:E:213:VAL:HG13	1:E:325:ILE:HB	1.90	0.53
1:F:225:LYS:HG2	1:F:226:LYS:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:PRO:HB3	1:B:272:LYS:HB2	1.89	0.53
1:G:348:GLN:HG2	1:G:352:GLN:HE21	1.74	0.53
1:C:213:VAL:HG13	1:C:325:ILE:HB	1.91	0.53
1:G:200:LEU:CD1	1:G:254:VAL:HB	2.38	0.53
1:C:77:VAL:HG21	1:C:510:VAL:HG13	1.88	0.53
1:C:348:GLN:HG2	1:C:352:GLN:HE21	1.74	0.53
1:A:411:VAL:HG21	1:A:494:LEU:HD13	1.91	0.53
1:C:225:LYS:HG2	1:C:226:LYS:N	2.24	0.53
1:D:69:MET:HE3	1:D:520:MET:HE2	1.90	0.53
1:D:220:ILE:HD12	1:D:248:LEU:HD23	1.90	0.53
1:D:225:LYS:HG2	1:D:226:LYS:N	2.24	0.53
1:E:362:ARG:O	1:E:366:GLN:HG2	2.08	0.53
1:F:190:VAL:HG22	1:F:191:GLU:N	2.23	0.53
1:B:287:ALA:O	1:B:290:GLN:HB3	2.09	0.53
1:B:342:ILE:O	1:B:346:VAL:HG23	2.09	0.53
1:F:348:GLN:HG2	1:F:352:GLN:HE21	1.74	0.53
1:A:225:LYS:HG2	1:A:226:LYS:N	2.23	0.52
1:B:69:MET:HE3	1:B:520:MET:HE2	1.90	0.52
1:B:348:GLN:HG2	1:B:352:GLN:HE21	1.75	0.52
1:C:219:PHE:O	1:C:247:LEU:HD12	2.08	0.52
1:E:158:VAL:O	1:E:162:ILE:HG12	2.10	0.52
1:F:200:LEU:CD1	1:F:254:VAL:HB	2.38	0.52
1:G:287:ALA:O	1:G:290:GLN:HB3	2.10	0.52
1:A:73:MET:HE3	1:B:49:ILE:HD11	1.91	0.52
1:C:511:ALA:O	1:C:515:ILE:HG13	2.08	0.52
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.91	0.52
1:F:194:GLN:HE21	1:F:331:THR:HB	1.73	0.52
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.91	0.52
1:G:219:PHE:O	1:G:247:LEU:HD12	2.09	0.52
1:G:194:GLN:HE21	1:G:331:THR:HB	1.74	0.52
1:B:225:LYS:HG2	1:B:226:LYS:N	2.23	0.52
1:D:178:GLU:HG2	1:D:322:ARG:NH2	2.25	0.52
1:E:194:GLN:HE21	1:E:331:THR:HB	1.73	0.52
1:D:146:GLN:O	1:D:150:ILE:HG13	2.10	0.52
1:G:472:GLY:HA3	1:G:476:TYR:CD2	2.45	0.52
1:A:348:GLN:HG2	1:A:352:GLN:HE21	1.75	0.52
1:C:158:VAL:O	1:C:162:ILE:HG12	2.10	0.52
1:D:213:VAL:HG13	1:D:325:ILE:HB	1.91	0.52
1:E:68:ASN:HD21	1:E:72:GLN:HE21	1.57	0.52
1:G:77:VAL:HG21	1:G:510:VAL:HG13	1.90	0.52
1:C:336:VAL:HG12	1:C:336:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.91	0.52
1:G:362:ARG:O	1:G:366:GLN:HG2	2.09	0.52
1:D:66:PHE:HA	1:D:69:MET:CE	2.40	0.52
1:D:186:GLU:HB2	1:D:380:LYS:HB2	1.91	0.52
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.92	0.52
1:E:77:VAL:HG21	1:E:510:VAL:HG13	1.91	0.52
1:E:348:GLN:HG2	1:E:352:GLN:HE21	1.75	0.52
1:C:66:PHE:HA	1:C:69:MET:CE	2.40	0.52
1:D:219:PHE:O	1:D:247:LEU:HD12	2.09	0.52
1:D:472:GLY:HA3	1:D:476:TYR:CD2	2.45	0.52
1:E:186:GLU:HB2	1:E:380:LYS:HB2	1.92	0.52
1:D:342:ILE:O	1:D:346:VAL:HG23	2.10	0.51
1:D:348:GLN:HG2	1:D:352:GLN:HE21	1.74	0.51
1:E:225:LYS:HG2	1:E:226:LYS:N	2.24	0.51
1:A:219:PHE:O	1:A:247:LEU:HD12	2.10	0.51
1:A:472:GLY:HA3	1:A:476:TYR:CD2	2.46	0.51
1:C:194:GLN:HE21	1:C:331:THR:HB	1.74	0.51
1:C:287:ALA:O	1:C:290:GLN:HB3	2.09	0.51
1:D:200:LEU:CD1	1:D:254:VAL:HB	2.39	0.51
1:D:362:ARG:O	1:D:366:GLN:HG2	2.10	0.51
1:F:213:VAL:HG13	1:F:325:ILE:HB	1.93	0.51
1:D:227:ILE:CG2	1:D:259:LEU:HD22	2.40	0.51
1:E:146:GLN:O	1:E:150:ILE:HG13	2.11	0.51
1:G:411:VAL:HG21	1:G:494:LEU:HD13	1.93	0.51
1:A:68:ASN:HD21	1:A:72:GLN:HE21	1.57	0.51
1:A:513:LEU:HD13	1:B:49:ILE:HD12	1.92	0.51
1:B:66:PHE:HA	1:B:69:MET:CE	2.41	0.51
1:C:321:LYS:HB3	1:C:334:ASP:HB3	1.92	0.51
1:E:287:ALA:O	1:E:290:GLN:HB3	2.11	0.51
1:C:254:VAL:HG12	1:C:260:ALA:HB2	1.93	0.51
1:F:140:ASP:OD2	1:F:142:LYS:HB2	2.11	0.51
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.93	0.51
1:B:140:ASP:OD2	1:B:142:LYS:HB2	2.09	0.51
1:F:254:VAL:HG12	1:F:260:ALA:HB2	1.92	0.51
1:F:411:VAL:HG21	1:F:494:LEU:HD13	1.93	0.51
1:C:41:ASP:O	1:C:42:LYS:HD3	2.11	0.51
1:E:124:VAL:O	1:E:128:VAL:HG23	2.10	0.51
1:E:219:PHE:O	1:E:247:LEU:HD12	2.10	0.51
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.92	0.51
1:A:49:ILE:HD12	1:G:513:LEU:HD13	1.93	0.51
1:A:287:ALA:O	1:A:290:GLN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:ILE:O	1:E:346:VAL:HG23	2.11	0.51
1:A:140:ASP:OD2	1:A:142:LYS:HB2	2.11	0.51
1:D:194:GLN:HE21	1:D:331:THR:HB	1.76	0.51
1:F:321:LYS:HB3	1:F:334:ASP:HB3	1.93	0.51
1:F:342:ILE:O	1:F:346:VAL:HG23	2.11	0.51
1:A:257:GLU:OE2	1:B:272:LYS:HE2	2.11	0.50
1:B:41:ASP:O	1:B:42:LYS:HD3	2.11	0.50
1:B:254:VAL:HG12	1:B:260:ALA:HB2	1.93	0.50
1:E:227:ILE:CG2	1:E:259:LEU:HD22	2.41	0.50
1:F:227:ILE:CG2	1:F:259:LEU:HD22	2.41	0.50
1:G:336:VAL:HG12	1:G:336:VAL:O	2.11	0.50
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.93	0.50
1:B:229:ASN:ND2	1:C:270:ILE:O	2.45	0.50
1:D:511:ALA:O	1:D:515:ILE:HG13	2.10	0.50
1:E:118:ARG:HD2	1:E:436:GLN:HE22	1.76	0.50
1:G:342:ILE:O	1:G:346:VAL:HG23	2.10	0.50
1:C:411:VAL:HG21	1:C:494:LEU:HD13	1.93	0.50
1:D:477:GLY:C	1:D:488:MET:HE3	2.37	0.50
1:A:200:LEU:CD1	1:A:254:VAL:HB	2.41	0.50
1:B:472:GLY:HA3	1:B:476:TYR:CD2	2.46	0.50
1:E:320:ALA:HA	1:E:334:ASP:O	2.11	0.50
1:B:227:ILE:CG2	1:B:259:LEU:HD22	2.41	0.50
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.92	0.50
1:E:101:THR:O	1:E:105:LYS:HG3	2.11	0.50
1:B:320:ALA:HA	1:B:334:ASP:O	2.12	0.50
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.93	0.50
1:C:146:GLN:O	1:C:150:ILE:HG13	2.11	0.50
1:C:227:ILE:CG2	1:C:259:LEU:HD22	2.42	0.50
1:C:227:ILE:CB	1:C:259:LEU:HD22	2.42	0.50
1:E:12:ALA:HB1	1:E:520:MET:HG3	1.94	0.50
1:E:411:VAL:HG21	1:E:494:LEU:HD13	1.94	0.50
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.93	0.50
1:G:284:ARG:HH11	1:G:284:ARG:HG3	1.77	0.50
1:A:254:VAL:HG12	1:A:260:ALA:HB2	1.93	0.50
1:A:321:LYS:HB3	1:A:334:ASP:HB3	1.94	0.50
1:A:362:ARG:O	1:A:366:GLN:HG2	2.12	0.50
1:C:320:ALA:HA	1:C:334:ASP:O	2.12	0.50
1:E:230:ILE:HD12	1:E:231:ARG:N	2.27	0.50
1:F:336:VAL:HG12	1:F:336:VAL:O	2.12	0.50
1:G:227:ILE:CB	1:G:259:LEU:HD22	2.42	0.50
1:A:146:GLN:O	1:A:150:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:THR:O	1:B:105:LYS:HG3	2.12	0.50
1:C:342:ILE:O	1:C:346:VAL:HG23	2.12	0.50
1:D:321:LYS:HB3	1:D:334:ASP:HB3	1.93	0.50
1:C:362:ARG:O	1:C:366:GLN:HG2	2.11	0.49
1:E:206:ASN:HB3	1:E:208:PRO:HD2	1.94	0.49
1:E:254:VAL:HG12	1:E:260:ALA:HB2	1.93	0.49
1:E:336:VAL:O	1:E:336:VAL:HG12	2.11	0.49
1:F:472:GLY:HA3	1:F:476:TYR:CD2	2.47	0.49
1:A:66:PHE:HA	1:A:69:MET:HE3	1.94	0.49
1:B:227:ILE:CB	1:B:259:LEU:HD22	2.41	0.49
1:D:254:VAL:HG12	1:D:260:ALA:HB2	1.93	0.49
1:E:321:LYS:HB3	1:E:334:ASP:HB3	1.94	0.49
1:F:206:ASN:HB3	1:F:208:PRO:HD2	1.94	0.49
1:G:227:ILE:CG2	1:G:259:LEU:HD22	2.42	0.49
1:G:254:VAL:HG12	1:G:260:ALA:HB2	1.94	0.49
1:A:49:ILE:HD11	1:G:73:MET:HE3	1.94	0.49
1:B:362:ARG:O	1:B:366:GLN:HG2	2.11	0.49
1:D:206:ASN:HB3	1:D:208:PRO:HD2	1.94	0.49
1:E:8:PHE:HE1	1:F:26:ALA:HA	1.77	0.49
1:F:226:LYS:HE3	1:F:253:ASP:HB3	1.94	0.49
1:A:230:ILE:HD12	1:A:231:ARG:N	2.27	0.49
1:A:284:ARG:NH2	1:B:182:GLY:HA2	2.27	0.49
1:D:142:LYS:HD3	1:D:142:LYS:N	2.27	0.49
1:G:140:ASP:OD2	1:G:142:LYS:HB2	2.12	0.49
1:G:142:LYS:N	1:G:142:LYS:HD3	2.27	0.49
1:B:321:LYS:HB3	1:B:334:ASP:HB3	1.95	0.49
1:C:206:ASN:HB3	1:C:208:PRO:HD2	1.94	0.49
1:D:158:VAL:O	1:D:162:ILE:HG12	2.13	0.49
1:D:230:ILE:HD12	1:D:231:ARG:N	2.27	0.49
1:D:404:ARG:O	1:D:407:VAL:HG22	2.12	0.49
1:D:411:VAL:HG21	1:D:494:LEU:HD13	1.95	0.49
1:E:41:ASP:O	1:E:42:LYS:HD3	2.12	0.49
1:G:68:ASN:HD21	1:G:72:GLN:HE21	1.61	0.49
1:C:477:GLY:C	1:C:488:MET:HE3	2.38	0.49
1:D:41:ASP:O	1:D:42:LYS:HD3	2.13	0.49
1:E:226:LYS:HE3	1:E:253:ASP:HB3	1.93	0.49
1:G:226:LYS:HE3	1:G:253:ASP:HB3	1.94	0.49
1:C:26:ALA:O	1:C:29:VAL:HG22	2.13	0.49
1:E:66:PHE:HA	1:E:69:MET:CE	2.43	0.49
1:F:41:ASP:O	1:F:42:LYS:HD3	2.12	0.49
1:F:68:ASN:HD21	1:F:72:GLN:HE21	1.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:ILE:CB	1:F:259:LEU:HD22	2.42	0.49
1:F:320:ALA:HA	1:F:334:ASP:O	2.13	0.49
1:G:12:ALA:HB1	1:G:520:MET:HG3	1.94	0.49
1:A:66:PHE:HA	1:A:69:MET:CE	2.43	0.49
1:B:284:ARG:HH11	1:B:284:ARG:HG3	1.78	0.49
1:C:226:LYS:HE3	1:C:253:ASP:HB3	1.94	0.49
1:C:448:GLU:O	1:C:452:ARG:HG3	2.12	0.49
1:D:227:ILE:CB	1:D:259:LEU:HD22	2.41	0.49
1:E:207:LYS:N	1:E:208:PRO:HD2	2.28	0.49
1:B:207:LYS:N	1:B:208:PRO:HD2	2.28	0.49
1:B:230:ILE:HD12	1:B:231:ARG:N	2.28	0.49
1:B:336:VAL:HG12	1:B:336:VAL:O	2.13	0.49
1:D:207:LYS:N	1:D:208:PRO:HD2	2.28	0.49
1:D:320:ALA:HA	1:D:334:ASP:O	2.12	0.49
1:G:146:GLN:O	1:G:150:ILE:HG13	2.12	0.49
1:G:448:GLU:O	1:G:452:ARG:HG3	2.12	0.49
1:A:206:ASN:HB3	1:A:208:PRO:HD2	1.95	0.49
1:A:336:VAL:HG12	1:A:336:VAL:O	2.11	0.49
1:B:206:ASN:HB3	1:B:208:PRO:HD2	1.95	0.49
1:C:142:LYS:HD3	1:C:142:LYS:N	2.28	0.49
1:C:284:ARG:HG3	1:C:284:ARG:HH11	1.78	0.49
1:D:136:VAL:HB	1:D:411:VAL:HG12	1.95	0.49
1:F:362:ARG:O	1:F:366:GLN:HG2	2.12	0.49
1:G:118:ARG:HD2	1:G:436:GLN:HE22	1.78	0.49
1:A:218:PRO:HD2	1:A:320:ALA:O	2.13	0.48
1:C:230:ILE:HD12	1:C:231:ARG:N	2.28	0.48
1:D:218:PRO:HD2	1:D:320:ALA:O	2.13	0.48
1:F:207:LYS:N	1:F:208:PRO:HD2	2.28	0.48
1:F:414:GLY:N	1:F:494:LEU:HA	2.28	0.48
1:G:190:VAL:HG22	1:G:191:GLU:N	2.27	0.48
1:A:90:THR:O	1:A:94:VAL:HG23	2.12	0.48
1:A:207:LYS:N	1:A:208:PRO:HD2	2.28	0.48
1:B:68:ASN:HD21	1:B:72:GLN:HE21	1.61	0.48
1:C:90:THR:O	1:C:94:VAL:HG23	2.12	0.48
1:F:158:VAL:O	1:F:162:ILE:HG12	2.13	0.48
1:G:230:ILE:HD12	1:G:231:ARG:N	2.27	0.48
1:B:12:ALA:HB1	1:B:520:MET:HG3	1.95	0.48
1:D:239:ALA:HB1	1:D:314:LEU:HG	1.96	0.48
1:E:227:ILE:CB	1:E:259:LEU:HD22	2.42	0.48
1:F:90:THR:O	1:F:94:VAL:HG23	2.13	0.48
1:F:284:ARG:HG3	1:F:284:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:VAL:O	1:G:162:ILE:HG12	2.13	0.48
1:C:207:LYS:N	1:C:208:PRO:HD2	2.28	0.48
1:D:193:MET:HG2	1:D:194:GLN:N	2.29	0.48
1:F:12:ALA:HB1	1:F:520:MET:HG3	1.96	0.48
1:G:321:LYS:HB3	1:G:334:ASP:HB3	1.96	0.48
1:A:226:LYS:HE3	1:A:253:ASP:HB3	1.94	0.48
1:A:227:ILE:CG2	1:A:259:LEU:HD22	2.43	0.48
1:B:217:SER:HA	1:B:320:ALA:O	2.13	0.48
1:B:511:ALA:O	1:B:515:ILE:HG13	2.13	0.48
1:D:336:VAL:HG12	1:D:336:VAL:O	2.13	0.48
1:G:207:LYS:N	1:G:208:PRO:HD2	2.28	0.48
1:B:77:VAL:HG11	1:B:510:VAL:HG22	1.95	0.48
1:B:226:LYS:HE3	1:B:253:ASP:HB3	1.95	0.48
1:B:239:ALA:HB1	1:B:314:LEU:HG	1.95	0.48
1:A:227:ILE:CB	1:A:259:LEU:HD22	2.42	0.48
1:A:511:ALA:O	1:A:515:ILE:HG13	2.14	0.48
1:F:118:ARG:HD2	1:F:436:GLN:HE22	1.78	0.48
1:G:206:ASN:HB3	1:G:208:PRO:HD2	1.95	0.48
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.96	0.48
1:E:477:GLY:C	1:E:488:MET:HE3	2.39	0.48
1:F:239:ALA:HB1	1:F:314:LEU:HG	1.96	0.48
1:A:239:ALA:HB1	1:A:314:LEU:HG	1.96	0.48
1:D:214:GLU:HG3	1:D:324:VAL:HG22	1.96	0.48
1:D:449:ALA:HB3	1:D:450:PRO:HD3	1.95	0.48
1:E:227:ILE:HG21	1:E:233:MET:HE3	1.96	0.48
1:F:230:ILE:HD12	1:F:231:ARG:N	2.28	0.48
1:E:511:ALA:O	1:E:515:ILE:HG13	2.13	0.47
1:G:101:THR:O	1:G:105:LYS:HG3	2.14	0.47
1:A:68:ASN:HD21	1:A:72:GLN:NE2	2.12	0.47
1:A:82:ASN:HB2	1:A:89:THR:OG1	2.14	0.47
1:A:158:VAL:O	1:A:162:ILE:HG12	2.14	0.47
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.80	0.47
1:C:217:SER:HA	1:C:320:ALA:O	2.15	0.47
1:C:472:GLY:HA3	1:C:476:TYR:CD2	2.50	0.47
1:D:101:THR:O	1:D:105:LYS:HG3	2.13	0.47
1:E:239:ALA:HB1	1:E:314:LEU:HG	1.96	0.47
1:F:217:SER:HA	1:F:320:ALA:O	2.13	0.47
1:F:511:ALA:O	1:F:515:ILE:HG13	2.14	0.47
1:G:227:ILE:HG21	1:G:233:MET:HE3	1.95	0.47
1:B:66:PHE:HA	1:B:69:MET:HE3	1.96	0.47
1:B:82:ASN:HB2	1:B:89:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:VAL:HG21	1:B:494:LEU:HD13	1.96	0.47
1:C:140:ASP:OD2	1:C:142:LYS:HB2	2.14	0.47
1:D:226:LYS:HE3	1:D:253:ASP:HB3	1.95	0.47
1:D:227:ILE:HG21	1:D:233:MET:HE3	1.96	0.47
1:E:140:ASP:OD2	1:E:142:LYS:HB2	2.15	0.47
1:F:82:ASN:HB2	1:F:89:THR:OG1	2.14	0.47
1:G:218:PRO:HD2	1:G:320:ALA:O	2.15	0.47
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.96	0.47
1:A:320:ALA:HA	1:A:334:ASP:O	2.15	0.47
1:E:284:ARG:HG3	1:E:284:ARG:HH11	1.80	0.47
1:B:158:VAL:O	1:B:162:ILE:HG12	2.14	0.47
1:B:218:PRO:HD2	1:B:320:ALA:O	2.14	0.47
1:C:393:LYS:O	1:C:397:GLU:HG3	2.14	0.47
1:D:140:ASP:OD2	1:D:142:LYS:HB2	2.15	0.47
1:D:284:ARG:HG3	1:D:284:ARG:HH11	1.79	0.47
1:E:217:SER:HA	1:E:320:ALA:O	2.13	0.47
1:E:218:PRO:HD2	1:E:320:ALA:O	2.15	0.47
1:A:69:MET:HE3	1:A:520:MET:HE2	1.96	0.47
1:B:227:ILE:HG21	1:B:233:MET:HE3	1.96	0.47
1:C:77:VAL:HG12	1:C:506:TYR:HB3	1.96	0.47
1:E:82:ASN:HB2	1:E:89:THR:OG1	2.15	0.47
1:F:101:THR:O	1:F:105:LYS:HG3	2.14	0.47
1:A:124:VAL:HG13	1:A:504:LEU:HD13	1.96	0.47
1:A:477:GLY:C	1:A:488:MET:HE3	2.39	0.47
1:C:77:VAL:HG11	1:C:510:VAL:HG22	1.97	0.47
1:C:124:VAL:O	1:C:128:VAL:HG23	2.15	0.47
1:C:227:ILE:HG21	1:C:233:MET:HE3	1.96	0.47
1:E:267:ILE:HG22	1:E:267:ILE:O	2.14	0.47
1:F:73:MET:HE3	1:G:49:ILE:CD1	2.45	0.47
1:A:77:VAL:HG12	1:A:506:TYR:HB3	1.95	0.47
1:A:142:LYS:HD3	1:A:142:LYS:N	2.30	0.47
1:A:231:ARG:HH22	1:B:244:GLY:HA2	1.79	0.47
1:E:214:GLU:HG3	1:E:324:VAL:HG22	1.97	0.47
1:E:479:ASN:O	1:E:483:GLU:N	2.47	0.47
1:G:77:VAL:HG12	1:G:506:TYR:HB3	1.96	0.47
1:C:82:ASN:HB2	1:C:89:THR:OG1	2.15	0.47
1:E:68:ASN:HD21	1:E:72:GLN:NE2	2.13	0.47
1:F:479:ASN:O	1:F:483:GLU:N	2.46	0.47
1:G:267:ILE:HG22	1:G:267:ILE:O	2.15	0.47
1:B:142:LYS:HD3	1:B:142:LYS:N	2.30	0.47
1:B:381:VAL:HG21	1:B:393:LYS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ALA:HB1	1:C:314:LEU:HG	1.96	0.47
1:G:239:ALA:HB1	1:G:314:LEU:HG	1.97	0.47
1:D:284:ARG:HH22	1:E:182:GLY:HA2	1.79	0.46
1:F:227:ILE:HG21	1:F:233:MET:HE3	1.96	0.46
1:F:284:ARG:CZ	1:G:182:GLY:HA2	2.46	0.46
1:G:414:GLY:N	1:G:494:LEU:HA	2.29	0.46
1:A:12:ALA:HB1	1:A:520:MET:HG3	1.96	0.46
1:C:101:THR:O	1:C:105:LYS:HG3	2.15	0.46
1:C:118:ARG:HD2	1:C:436:GLN:HE22	1.80	0.46
1:C:229:ASN:ND2	1:D:270:ILE:HA	2.30	0.46
1:C:193:MET:HG2	1:C:194:GLN:N	2.29	0.46
1:C:414:GLY:N	1:C:494:LEU:HA	2.30	0.46
1:F:193:MET:HG2	1:F:194:GLN:N	2.30	0.46
1:A:101:THR:O	1:A:105:LYS:HG3	2.14	0.46
1:A:267:ILE:HG22	1:A:267:ILE:O	2.15	0.46
1:A:404:ARG:O	1:A:407:VAL:HG22	2.16	0.46
1:A:414:GLY:N	1:A:494:LEU:HA	2.31	0.46
1:D:414:GLY:N	1:D:494:LEU:HA	2.30	0.46
1:E:77:VAL:HG12	1:E:506:TYR:HB3	1.97	0.46
1:E:393:LYS:O	1:E:397:GLU:HG3	2.15	0.46
1:F:214:GLU:HG3	1:F:324:VAL:HG22	1.97	0.46
1:F:404:ARG:O	1:F:407:VAL:HG22	2.15	0.46
1:F:452:ARG:NH2	1:F:463:SER:HB3	2.31	0.46
1:B:146:GLN:O	1:B:150:ILE:HG13	2.16	0.46
1:B:270:ILE:HG23	1:B:271:VAL:HG23	1.97	0.46
1:D:68:ASN:HD21	1:D:72:GLN:HE21	1.63	0.46
1:D:118:ARG:HD2	1:D:436:GLN:HE22	1.80	0.46
1:B:77:VAL:HG12	1:B:506:TYR:HB3	1.97	0.46
1:B:267:ILE:O	1:B:267:ILE:HG22	2.15	0.46
1:D:4:LYS:HE2	1:E:59:GLU:O	2.15	0.46
1:F:66:PHE:HA	1:F:69:MET:CE	2.45	0.46
1:F:218:PRO:HD2	1:F:320:ALA:O	2.16	0.46
1:F:282:GLY:HA3	1:G:181:THR:O	2.15	0.46
1:A:228:SER:HB3	1:A:255:GLU:CD	2.41	0.46
1:A:411:VAL:CG2	1:A:494:LEU:HD13	2.45	0.46
1:D:82:ASN:HB2	1:D:89:THR:OG1	2.15	0.46
1:D:217:SER:HA	1:D:320:ALA:O	2.16	0.46
1:E:193:MET:HG2	1:E:194:GLN:N	2.31	0.46
1:A:227:ILE:HG21	1:A:233:MET:HE3	1.97	0.46
1:A:284:ARG:HH22	1:B:182:GLY:HA2	1.81	0.46
1:D:190:VAL:HG13	1:D:333:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:SER:CB	1:E:255:GLU:HB2	2.45	0.46
1:F:142:LYS:HD3	1:F:142:LYS:N	2.31	0.46
1:G:66:PHE:HA	1:G:69:MET:CE	2.45	0.46
1:G:217:SER:HA	1:G:320:ALA:O	2.15	0.46
1:G:228:SER:HB3	1:G:255:GLU:CD	2.41	0.46
1:G:320:ALA:HA	1:G:334:ASP:O	2.16	0.46
1:A:228:SER:CB	1:A:255:GLU:HB2	2.45	0.46
1:A:271:VAL:HG12	1:A:272:LYS:H	1.81	0.46
1:E:381:VAL:HG21	1:E:393:LYS:HA	1.98	0.46
1:F:68:ASN:HD21	1:F:72:GLN:NE2	2.13	0.46
1:G:271:VAL:HG12	1:G:272:LYS:H	1.81	0.46
1:A:2:ALA:O	1:A:3:ALA:C	2.59	0.46
1:A:183:LEU:HA	1:A:383:ALA:O	2.16	0.46
1:A:214:GLU:HG3	1:A:324:VAL:HG22	1.98	0.46
1:A:448:GLU:O	1:A:452:ARG:HG3	2.16	0.46
1:A:479:ASN:O	1:A:483:GLU:N	2.48	0.46
1:D:12:ALA:HB1	1:D:520:MET:HG3	1.97	0.46
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.15	0.46
1:A:8:PHE:HA	1:A:518:GLU:O	2.16	0.45
1:A:193:MET:HG2	1:A:194:GLN:N	2.30	0.45
1:A:217:SER:HA	1:A:320:ALA:O	2.15	0.45
1:B:271:VAL:HG12	1:B:272:LYS:H	1.81	0.45
1:C:345:ARG:HA	1:C:345:ARG:HD3	1.66	0.45
1:D:465:VAL:O	1:D:469:VAL:HG23	2.16	0.45
1:B:414:GLY:N	1:B:494:LEU:HA	2.31	0.45
1:C:381:VAL:HG21	1:C:393:LYS:HA	1.98	0.45
1:F:381:VAL:HG21	1:F:393:LYS:HA	1.98	0.45
1:B:193:MET:HG2	1:B:194:GLN:N	2.30	0.45
1:B:345:ARG:HA	1:B:345:ARG:HD3	1.67	0.45
1:D:267:ILE:O	1:D:267:ILE:HG22	2.16	0.45
1:C:218:PRO:O	1:C:319:GLN:HG3	2.17	0.45
1:C:228:SER:HB3	1:C:255:GLU:CD	2.41	0.45
1:C:479:ASN:O	1:C:483:GLU:N	2.47	0.45
1:D:270:ILE:HG23	1:D:271:VAL:HG23	1.97	0.45
1:D:479:ASN:O	1:D:483:GLU:N	2.50	0.45
1:C:270:ILE:HG23	1:C:271:VAL:HG23	1.99	0.45
1:E:472:GLY:HA3	1:E:476:TYR:CD2	2.52	0.45
1:F:77:VAL:HG12	1:F:506:TYR:HB3	1.97	0.45
1:F:190:VAL:HG22	1:F:191:GLU:H	1.81	0.45
1:F:271:VAL:HG12	1:F:272:LYS:H	1.81	0.45
1:G:193:MET:HG2	1:G:194:GLN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:SER:CB	1:G:255:GLU:HB2	2.46	0.45
1:G:230:ILE:HG22	1:G:259:LEU:HD12	1.99	0.45
1:G:411:VAL:CG2	1:G:494:LEU:HD13	2.46	0.45
1:C:214:GLU:HG3	1:C:324:VAL:HG22	1.98	0.45
1:C:411:VAL:CG2	1:C:494:LEU:HD13	2.46	0.45
1:D:66:PHE:HA	1:D:69:MET:HE3	1.99	0.45
1:E:414:GLY:N	1:E:494:LEU:HA	2.32	0.45
1:F:477:GLY:C	1:F:488:MET:HE3	2.41	0.45
1:A:270:ILE:HG23	1:A:271:VAL:HG23	1.98	0.45
1:B:118:ARG:HD2	1:B:436:GLN:HE22	1.82	0.45
1:D:360:TYR:O	1:D:364:LYS:HG2	2.17	0.45
1:A:49:ILE:CD1	1:G:73:MET:HE3	2.46	0.45
1:B:7:LYS:O	1:B:519:CYS:HA	2.16	0.45
1:B:271:VAL:HG12	1:B:272:LYS:N	2.32	0.45
1:B:448:GLU:O	1:B:452:ARG:HG3	2.16	0.45
1:B:513:LEU:HD13	1:C:49:ILE:HD12	1.98	0.45
1:C:66:PHE:HA	1:C:69:MET:HE3	1.99	0.45
1:C:267:ILE:HG22	1:C:267:ILE:O	2.16	0.45
1:F:218:PRO:O	1:F:319:GLN:HG3	2.17	0.45
1:F:267:ILE:O	1:F:267:ILE:HG22	2.16	0.45
1:G:270:ILE:HG23	1:G:271:VAL:HG23	1.98	0.45
1:G:472:GLY:HA3	1:G:476:TYR:HD2	1.82	0.45
1:B:479:ASN:O	1:B:483:GLU:N	2.48	0.45
1:D:77:VAL:HG12	1:D:506:TYR:HB3	1.98	0.45
1:E:142:LYS:HD3	1:E:142:LYS:N	2.31	0.45
1:G:479:ASN:O	1:G:483:GLU:N	2.50	0.45
1:A:73:MET:HE3	1:B:49:ILE:CD1	2.47	0.45
1:B:228:SER:CB	1:B:255:GLU:HB2	2.46	0.45
1:C:68:ASN:HD21	1:C:72:GLN:HE21	1.64	0.45
1:D:271:VAL:HG12	1:D:272:LYS:H	1.81	0.45
1:G:77:VAL:HG11	1:G:510:VAL:HG22	1.99	0.45
1:G:345:ARG:HD3	1:G:345:ARG:HA	1.64	0.45
1:G:477:GLY:C	1:G:488:MET:HE3	2.42	0.45
1:C:7:LYS:O	1:C:519:CYS:HA	2.16	0.44
1:C:228:SER:CB	1:C:255:GLU:HB2	2.45	0.44
1:D:228:SER:HB3	1:D:255:GLU:CD	2.42	0.44
1:E:228:SER:HB3	1:E:255:GLU:CD	2.42	0.44
1:E:271:VAL:HG12	1:E:272:LYS:H	1.82	0.44
1:F:228:SER:HB3	1:F:255:GLU:CD	2.42	0.44
1:F:228:SER:CB	1:F:255:GLU:HB2	2.45	0.44
1:A:271:VAL:HG12	1:A:272:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ASN:ND2	1:B:493:ILE:HD11	2.32	0.44
1:D:124:VAL:O	1:D:128:VAL:HG23	2.17	0.44
1:D:345:ARG:HA	1:D:345:ARG:HD3	1.65	0.44
1:E:271:VAL:HG12	1:E:272:LYS:N	2.33	0.44
1:B:8:PHE:HA	1:B:518:GLU:O	2.18	0.44
1:B:218:PRO:O	1:B:319:GLN:HG3	2.17	0.44
1:F:174:VAL:HG22	1:F:376:VAL:HG13	1.99	0.44
1:F:270:ILE:HG23	1:F:271:VAL:HG23	1.98	0.44
1:F:448:GLU:O	1:F:452:ARG:HG3	2.17	0.44
1:F:465:VAL:O	1:F:469:VAL:HG23	2.17	0.44
1:B:90:THR:O	1:B:94:VAL:HG23	2.17	0.44
1:B:466:ALA:O	1:B:470:LYS:HG3	2.17	0.44
1:C:142:LYS:O	1:C:146:GLN:HG3	2.18	0.44
1:C:209:GLU:CD	1:C:209:GLU:H	2.26	0.44
1:C:465:VAL:O	1:C:469:VAL:HG23	2.17	0.44
1:C:230:ILE:HG22	1:C:259:LEU:HD12	1.99	0.44
1:F:393:LYS:O	1:F:397:GLU:HG3	2.18	0.44
1:A:360:TYR:O	1:A:364:LYS:HG2	2.17	0.44
1:A:465:VAL:O	1:A:469:VAL:HG23	2.16	0.44
1:B:26:ALA:O	1:B:29:VAL:HG22	2.17	0.44
1:B:152:ALA:HB2	1:B:158:VAL:HG11	2.00	0.44
1:C:218:PRO:HD2	1:C:320:ALA:O	2.17	0.44
1:D:90:THR:O	1:D:94:VAL:HG23	2.18	0.44
1:E:345:ARG:HA	1:E:345:ARG:HD3	1.67	0.44
1:G:190:VAL:HG22	1:G:191:GLU:H	1.83	0.44
1:C:271:VAL:HG12	1:C:272:LYS:H	1.82	0.44
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.99	0.44
1:E:230:ILE:HG22	1:E:259:LEU:HD12	2.00	0.44
1:E:381:VAL:O	1:E:389:MET:HG2	2.18	0.44
1:G:183:LEU:HA	1:G:383:ALA:O	2.17	0.44
1:G:393:LYS:O	1:G:397:GLU:HG3	2.18	0.44
1:B:228:SER:HB3	1:B:255:GLU:CD	2.42	0.44
1:B:281:PHE:HB3	1:C:386:GLU:OE1	2.18	0.44
1:B:360:TYR:O	1:B:364:LYS:HG2	2.17	0.44
1:D:230:ILE:HG22	1:D:259:LEU:HD12	2.00	0.44
1:E:514:MET:HE3	1:E:514:MET:HB2	1.89	0.44
1:F:166:MET:O	1:F:170:GLY:N	2.51	0.44
1:F:271:VAL:HG12	1:F:272:LYS:N	2.32	0.44
1:A:41:ASP:O	1:A:42:LYS:HD3	2.18	0.44
1:A:230:ILE:HG22	1:A:259:LEU:HD12	2.00	0.44
1:B:68:ASN:HD21	1:B:72:GLN:NE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLU:HG3	1:B:324:VAL:HG22	1.99	0.44
1:C:360:TYR:O	1:C:364:LYS:HG2	2.18	0.44
1:D:271:VAL:HG12	1:D:272:LYS:N	2.32	0.44
1:D:393:LYS:O	1:D:397:GLU:HG3	2.18	0.44
1:D:514:MET:HE3	1:D:514:MET:HB2	1.93	0.44
1:E:26:ALA:O	1:E:29:VAL:HG22	2.18	0.44
1:E:360:TYR:O	1:E:364:LYS:HG2	2.18	0.44
1:F:8:PHE:HA	1:F:518:GLU:O	2.18	0.44
1:F:411:VAL:CG2	1:F:494:LEU:HD13	2.47	0.44
1:G:68:ASN:HD21	1:G:72:GLN:NE2	2.16	0.44
1:G:213:VAL:CG1	1:G:325:ILE:HB	2.48	0.44
1:A:26:ALA:O	1:A:29:VAL:HG22	2.17	0.43
1:B:16:MET:SD	1:B:514:MET:HG3	2.58	0.43
1:B:183:LEU:HA	1:B:383:ALA:O	2.17	0.43
1:B:213:VAL:CG1	1:B:325:ILE:HB	2.48	0.43
1:F:360:TYR:O	1:F:364:LYS:HG2	2.17	0.43
1:G:271:VAL:HG12	1:G:272:LYS:N	2.32	0.43
1:A:152:ALA:HB2	1:A:158:VAL:HG11	2.00	0.43
1:B:2:ALA:O	1:B:3:ALA:C	2.60	0.43
1:B:414:GLY:HA2	1:B:495:ASP:OD2	2.18	0.43
1:C:8:PHE:HA	1:C:518:GLU:O	2.18	0.43
1:C:183:LEU:HA	1:C:383:ALA:O	2.18	0.43
1:E:111:MET:O	1:E:113:PRO:HD3	2.18	0.43
1:A:209:GLU:CD	1:A:209:GLU:H	2.27	0.43
1:B:192:GLY:HA3	1:B:376:VAL:HG23	2.00	0.43
1:G:124:VAL:O	1:G:128:VAL:HG23	2.18	0.43
1:A:213:VAL:CG1	1:A:325:ILE:HB	2.48	0.43
1:B:124:VAL:HG13	1:B:504:LEU:HD13	1.99	0.43
1:C:420:ILE:HG12	1:C:470:LYS:HG2	2.00	0.43
1:D:218:PRO:O	1:D:319:GLN:HG3	2.18	0.43
1:F:230:ILE:HG22	1:F:259:LEU:HD12	2.01	0.43
1:A:218:PRO:O	1:A:319:GLN:HG3	2.18	0.43
1:B:142:LYS:O	1:B:146:GLN:HG3	2.19	0.43
1:D:228:SER:CB	1:D:255:GLU:HB2	2.45	0.43
1:F:345:ARG:HD3	1:F:345:ARG:HA	1.65	0.43
1:G:166:MET:O	1:G:170:GLY:N	2.51	0.43
1:G:191:GLU:O	1:G:334:ASP:HA	2.19	0.43
1:G:214:GLU:HG3	1:G:324:VAL:HG22	1.99	0.43
1:B:230:ILE:HG22	1:B:259:LEU:HD12	2.01	0.43
1:E:404:ARG:O	1:E:407:VAL:HG22	2.19	0.43
1:G:465:VAL:O	1:G:469:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:O	1:A:334:ASP:HA	2.18	0.43
1:A:472:GLY:HA3	1:A:476:TYR:HD2	1.84	0.43
1:C:12:ALA:HB1	1:C:520:MET:HG3	2.01	0.43
1:D:68:ASN:HD21	1:D:72:GLN:NE2	2.17	0.43
1:E:215:LEU:O	1:E:218:PRO:HD3	2.18	0.43
1:F:215:LEU:O	1:F:218:PRO:HD3	2.18	0.43
1:G:360:TYR:O	1:G:364:LYS:HG2	2.18	0.43
1:G:514:MET:HE3	1:G:514:MET:HB2	1.95	0.43
1:A:519:CYS:HB3	1:B:38:VAL:HG22	2.00	0.43
1:C:2:ALA:O	1:C:3:ALA:C	2.61	0.43
1:C:414:GLY:HA2	1:C:495:ASP:OD2	2.18	0.43
1:E:270:ILE:HG23	1:E:271:VAL:HG23	1.99	0.43
1:E:324:VAL:HB	1:E:331:THR:HG22	2.01	0.43
1:F:73:MET:HE3	1:G:49:ILE:HD11	2.01	0.43
1:G:230:ILE:CG2	1:G:259:LEU:HD12	2.49	0.43
1:A:393:LYS:O	1:A:397:GLU:HG3	2.19	0.43
1:C:271:VAL:HG12	1:C:272:LYS:N	2.32	0.43
1:E:209:GLU:H	1:E:209:GLU:CD	2.27	0.43
1:F:2:ALA:O	1:F:3:ALA:C	2.61	0.43
1:F:183:LEU:HA	1:F:383:ALA:O	2.19	0.43
1:F:411:VAL:HG11	1:F:494:LEU:HD22	2.01	0.43
1:A:142:LYS:O	1:A:146:GLN:HG3	2.19	0.43
1:D:117:LYS:NZ	2:D:550:HOH:O	2.52	0.43
1:D:472:GLY:HA3	1:D:476:TYR:HD2	1.84	0.43
1:E:383:ALA:HB3	1:E:389:MET:HB2	2.00	0.43
1:F:26:ALA:O	1:F:29:VAL:HG22	2.18	0.43
1:F:209:GLU:CD	1:F:209:GLU:H	2.27	0.43
1:F:324:VAL:HB	1:F:331:THR:HG22	2.00	0.43
1:A:421:ARG:CD	1:A:474:GLY:O	2.67	0.42
1:D:7:LYS:O	1:D:519:CYS:HA	2.18	0.42
1:D:324:VAL:HB	1:D:331:THR:HG22	2.01	0.42
1:G:209:GLU:H	1:G:209:GLU:CD	2.27	0.42
1:A:124:VAL:O	1:A:128:VAL:HG23	2.18	0.42
1:D:183:LEU:HA	1:D:383:ALA:O	2.19	0.42
1:D:452:ARG:NH2	1:D:463:SER:HB3	2.33	0.42
1:A:118:ARG:HD2	1:A:436:GLN:HE22	1.83	0.42
1:B:191:GLU:O	1:B:334:ASP:HA	2.19	0.42
1:D:142:LYS:O	1:D:146:GLN:HG3	2.19	0.42
1:E:183:LEU:HA	1:E:383:ALA:O	2.19	0.42
1:A:386:GLU:OE1	1:G:281:PHE:HB3	2.20	0.42
1:A:421:ARG:HD3	1:A:474:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:MET:O	1:B:113:PRO:HD3	2.20	0.42
1:D:152:ALA:HB2	1:D:158:VAL:HG11	2.01	0.42
1:E:90:THR:O	1:E:94:VAL:HG23	2.18	0.42
1:E:142:LYS:O	1:E:146:GLN:HG3	2.19	0.42
1:F:461:GLU:HA	1:F:462:PRO:HD2	1.94	0.42
1:G:142:LYS:O	1:G:146:GLN:HG3	2.19	0.42
1:C:215:LEU:O	1:C:218:PRO:HD3	2.18	0.42
1:F:466:ALA:O	1:F:470:LYS:HG3	2.19	0.42
1:G:452:ARG:NH2	1:G:463:SER:HB3	2.35	0.42
1:A:7:LYS:O	1:A:519:CYS:HA	2.19	0.42
1:B:166:MET:O	1:B:170:GLY:N	2.53	0.42
1:E:7:LYS:O	1:E:519:CYS:HA	2.19	0.42
1:E:213:VAL:CG1	1:E:325:ILE:HB	2.49	0.42
1:E:230:ILE:CG2	1:E:259:LEU:HD12	2.50	0.42
1:B:324:VAL:HB	1:B:331:THR:HG22	2.01	0.42
1:C:213:VAL:CG1	1:C:325:ILE:HB	2.50	0.42
1:D:26:ALA:O	1:D:29:VAL:HG22	2.19	0.42
1:E:66:PHE:HA	1:E:69:MET:HE3	2.02	0.42
1:E:118:ARG:HH11	1:E:436:GLN:NE2	2.17	0.42
1:F:414:GLY:HA2	1:F:495:ASP:OD2	2.20	0.42
1:G:215:LEU:O	1:G:218:PRO:HD3	2.20	0.42
1:G:218:PRO:O	1:G:319:GLN:HG3	2.19	0.42
1:A:420:ILE:HG12	1:A:470:LYS:HG2	2.00	0.42
1:B:393:LYS:O	1:B:397:GLU:HG3	2.19	0.42
1:D:2:ALA:O	1:D:3:ALA:C	2.61	0.42
1:D:209:GLU:CD	1:D:209:GLU:H	2.26	0.42
1:D:411:VAL:CG2	1:D:494:LEU:HD13	2.49	0.42
1:F:230:ILE:H	1:F:230:ILE:HG13	1.68	0.42
1:A:215:LEU:O	1:A:218:PRO:HD3	2.19	0.42
1:B:413:ALA:HB2	1:B:475:ASN:OD1	2.20	0.42
1:D:8:PHE:HA	1:D:518:GLU:O	2.20	0.42
1:D:230:ILE:CG2	1:D:259:LEU:HD12	2.50	0.42
1:E:16:MET:SD	1:E:514:MET:HG3	2.60	0.42
1:E:218:PRO:O	1:E:319:GLN:HG3	2.20	0.42
1:F:152:ALA:HB2	1:F:158:VAL:HG11	2.02	0.42
1:G:8:PHE:HA	1:G:518:GLU:O	2.20	0.42
1:G:124:VAL:HG13	1:G:504:LEU:HD13	2.00	0.42
1:D:414:GLY:HA2	1:D:495:ASP:OD2	2.20	0.42
1:E:420:ILE:HG12	1:E:470:LYS:HG2	2.02	0.42
1:G:152:ALA:HB2	1:G:158:VAL:HG11	2.02	0.42
1:C:404:ARG:O	1:C:407:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:GLU:OE1	1:F:269:GLY:HA2	2.20	0.41
1:E:411:VAL:HG11	1:E:494:LEU:HD22	2.01	0.41
1:F:33:PRO:C	1:F:34:LYS:HD2	2.45	0.41
1:F:124:VAL:O	1:F:128:VAL:HG23	2.20	0.41
1:G:421:ARG:HD3	1:G:474:GLY:O	2.20	0.41
1:A:452:ARG:NH2	1:A:463:SER:HB3	2.36	0.41
1:A:461:GLU:HA	1:A:462:PRO:HD2	1.96	0.41
1:C:73:MET:HE3	1:D:49:ILE:CD1	2.50	0.41
1:E:335:GLY:C	1:E:337:GLY:H	2.29	0.41
1:B:472:GLY:HA3	1:B:476:TYR:HD2	1.85	0.41
1:D:203:TYR:CD1	1:D:203:TYR:N	2.88	0.41
1:D:215:LEU:O	1:D:218:PRO:HD3	2.20	0.41
1:D:479:ASN:ND2	1:D:493:ILE:HD11	2.35	0.41
1:E:124:VAL:HG13	1:E:504:LEU:HD13	2.01	0.41
1:F:412:VAL:HG13	1:F:497:THR:OG1	2.20	0.41
1:C:68:ASN:HD21	1:C:72:GLN:NE2	2.18	0.41
1:C:190:VAL:HG22	1:C:191:GLU:H	1.81	0.41
1:G:324:VAL:HB	1:G:331:THR:HG22	2.01	0.41
1:A:335:GLY:C	1:A:337:GLY:H	2.29	0.41
1:B:477:GLY:C	1:B:488:MET:HE3	2.45	0.41
1:B:514:MET:HE3	1:B:514:MET:HB2	1.99	0.41
1:C:230:ILE:CG2	1:C:259:LEU:HD12	2.50	0.41
1:D:77:VAL:HG11	1:D:510:VAL:HG22	2.03	0.41
1:D:283:ASP:HA	1:D:286:LYS:HE2	2.02	0.41
1:D:421:ARG:HD3	1:D:474:GLY:O	2.20	0.41
1:E:414:GLY:HA2	1:E:495:ASP:OD2	2.20	0.41
1:G:479:ASN:ND2	1:G:493:ILE:HD11	2.36	0.41
1:A:381:VAL:O	1:A:389:MET:HG2	2.21	0.41
1:B:411:VAL:HG11	1:B:494:LEU:HD22	2.02	0.41
1:C:111:MET:O	1:C:113:PRO:HD3	2.21	0.41
1:C:152:ALA:HB2	1:C:158:VAL:HG11	2.02	0.41
1:D:420:ILE:HG12	1:D:470:LYS:HG2	2.02	0.41
1:D:421:ARG:CD	1:D:474:GLY:O	2.68	0.41
1:E:466:ALA:O	1:E:470:LYS:HG3	2.20	0.41
1:F:146:GLN:O	1:F:150:ILE:HG13	2.20	0.41
1:F:230:ILE:CG2	1:F:259:LEU:HD12	2.51	0.41
1:G:90:THR:O	1:G:94:VAL:HG23	2.20	0.41
1:G:283:ASP:HA	1:G:286:LYS:HE2	2.02	0.41
1:A:324:VAL:HB	1:A:331:THR:HG22	2.02	0.41
1:B:19:GLY:HA3	1:B:67:GLU:O	2.21	0.41
1:B:438:VAL:O	1:B:442:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:VAL:HB	1:C:331:THR:HG22	2.02	0.41
1:D:191:GLU:O	1:D:334:ASP:HA	2.19	0.41
1:D:213:VAL:CG1	1:D:325:ILE:HB	2.50	0.41
1:G:66:PHE:HA	1:G:69:MET:HE3	2.03	0.41
1:A:230:ILE:CG2	1:A:259:LEU:HD12	2.50	0.41
1:A:438:VAL:O	1:A:442:VAL:HG23	2.20	0.41
1:B:335:GLY:C	1:B:337:GLY:H	2.28	0.41
1:B:404:ARG:O	1:B:407:VAL:HG22	2.19	0.41
1:B:461:GLU:HA	1:B:462:PRO:HD2	1.94	0.41
1:C:191:GLU:O	1:C:334:ASP:HA	2.20	0.41
1:C:203:TYR:N	1:C:203:TYR:CD1	2.89	0.41
1:D:519:CYS:HB3	1:E:38:VAL:HG22	2.03	0.41
1:F:213:VAL:CG1	1:F:325:ILE:HB	2.51	0.41
1:B:112:ASN:HD22	1:C:459:GLY:HA3	1.84	0.41
1:B:230:ILE:CG2	1:B:259:LEU:HD12	2.50	0.41
1:C:452:ARG:NH2	1:C:463:SER:HB3	2.36	0.41
1:E:461:GLU:HA	1:E:462:PRO:HD2	1.96	0.41
1:G:26:ALA:O	1:G:29:VAL:HG22	2.21	0.41
1:G:381:VAL:O	1:G:389:MET:HG2	2.21	0.41
1:G:411:VAL:HG11	1:G:494:LEU:HD22	2.02	0.41
1:G:414:GLY:H	1:G:494:LEU:HA	1.86	0.41
1:G:466:ALA:O	1:G:470:LYS:HG3	2.21	0.41
1:C:19:GLY:HA3	1:C:67:GLU:O	2.21	0.41
1:C:421:ARG:HD3	1:C:474:GLY:O	2.21	0.41
1:D:321:LYS:HB2	1:D:334:ASP:HB3	2.03	0.41
1:D:335:GLY:C	1:D:337:GLY:H	2.29	0.41
1:D:383:ALA:HB3	1:D:389:MET:HB2	2.02	0.41
1:B:132:LYS:HE3	1:B:132:LYS:HB2	1.94	0.40
1:D:166:MET:O	1:D:170:GLY:N	2.54	0.40
1:E:152:ALA:HB2	1:E:158:VAL:HG11	2.02	0.40
1:E:452:ARG:NH2	1:E:463:SER:HB3	2.36	0.40
1:F:203:TYR:CD1	1:F:203:TYR:N	2.89	0.40
1:A:455:VAL:HG13	1:A:460:GLU:HB2	2.04	0.40
1:C:414:GLY:H	1:C:494:LEU:HA	1.87	0.40
1:E:197:ARG:HE	1:E:279:PRO:HA	1.86	0.40
1:F:66:PHE:HA	1:F:69:MET:HE3	2.03	0.40
1:F:77:VAL:HG11	1:F:510:VAL:HG22	2.02	0.40
1:F:455:VAL:HG13	1:F:460:GLU:HB2	2.03	0.40
1:G:203:TYR:CD1	1:G:203:TYR:N	2.89	0.40
1:B:283:ASP:HA	1:B:286:LYS:HE2	2.02	0.40
1:B:455:VAL:HG13	1:B:460:GLU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ASP:OD2	1:C:142:LYS:HE2	2.22	0.40
1:C:197:ARG:HE	1:C:279:PRO:HA	1.86	0.40
1:D:118:ARG:HH11	1:D:436:GLN:NE2	2.19	0.40
1:E:434:GLU:O	1:E:438:VAL:HG13	2.21	0.40
1:F:118:ARG:HH11	1:F:436:GLN:NE2	2.19	0.40
1:G:335:GLY:C	1:G:337:GLY:H	2.29	0.40
1:A:126:VAL:O	1:A:129:GLU:HB2	2.22	0.40
1:B:140:ASP:OD2	1:B:142:LYS:HE2	2.21	0.40
1:B:421:ARG:HD3	1:B:474:GLY:O	2.21	0.40
1:C:438:VAL:O	1:C:442:VAL:HG23	2.21	0.40
1:G:19:GLY:HA3	1:G:67:GLU:O	2.21	0.40
1:G:383:ALA:HB3	1:G:389:MET:HB2	2.02	0.40
1:A:33:PRO:C	1:A:34:LYS:HD2	2.47	0.40
1:A:283:ASP:HA	1:A:286:LYS:HE2	2.03	0.40
1:A:514:MET:HE3	1:A:514:MET:HB2	2.00	0.40
1:C:229:ASN:HD21	1:D:270:ILE:HA	1.85	0.40
1:C:305:ILE:O	1:C:305:ILE:HG22	2.22	0.40
1:C:461:GLU:HA	1:C:462:PRO:HD2	1.96	0.40
1:C:514:MET:HE3	1:C:514:MET:HB2	1.95	0.40
1:D:19:GLY:HA3	1:D:67:GLU:O	2.21	0.40
1:D:126:VAL:O	1:D:129:GLU:HB2	2.21	0.40
1:D:443:ALA:O	1:D:447:MET:HG3	2.22	0.40
1:E:136:VAL:HB	1:E:411:VAL:HG12	2.04	0.40
1:E:191:GLU:O	1:E:334:ASP:HA	2.21	0.40
1:E:203:TYR:CD1	1:E:203:TYR:N	2.90	0.40
1:E:284:ARG:NH1	1:F:182:GLY:HA2	2.36	0.40
1:F:191:GLU:O	1:F:334:ASP:HA	2.22	0.40
1:F:414:GLY:H	1:F:494:LEU:HA	1.87	0.40
1:G:404:ARG:O	1:G:407:VAL:HG22	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	522/547 (95%)	497 (95%)	23 (4%)	2 (0%)	30	60
1	B	522/547 (95%)	498 (95%)	22 (4%)	2 (0%)	30	60
1	C	522/547 (95%)	496 (95%)	24 (5%)	2 (0%)	30	60
1	D	522/547 (95%)	497 (95%)	23 (4%)	2 (0%)	30	60
1	E	522/547 (95%)	497 (95%)	24 (5%)	1 (0%)	43	72
1	F	522/547 (95%)	497 (95%)	22 (4%)	3 (1%)	21	51
1	G	522/547 (95%)	497 (95%)	24 (5%)	1 (0%)	43	72
All	All	3654/3829 (95%)	3479 (95%)	162 (4%)	13 (0%)	30	60

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	426	LEU
1	C	426	LEU
1	C	269	GLY
1	E	269	GLY
1	F	269	GLY
1	G	269	GLY
1	A	269	GLY
1	B	269	GLY
1	D	269	GLY
1	A	336	VAL
1	B	336	VAL
1	D	336	VAL
1	F	336	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	403/413 (98%)	388 (96%)	15 (4%)	30	65
1	B	403/413 (98%)	388 (96%)	15 (4%)	30	65
1	C	403/413 (98%)	387 (96%)	16 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	403/413 (98%)	387 (96%)	16 (4%)	28	63
1	E	403/413 (98%)	387 (96%)	16 (4%)	28	63
1	F	403/413 (98%)	388 (96%)	15 (4%)	30	65
1	G	403/413 (98%)	387 (96%)	16 (4%)	28	63
All	All	2821/2891 (98%)	2712 (96%)	109 (4%)	28	64

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	116	LEU
1	A	174	VAL
1	A	213	VAL
1	A	214	GLU
1	A	230	ILE
1	A	232	GLU
1	A	290	GLN
1	A	328	ASP
1	A	345	ARG
1	A	411	VAL
1	A	438	VAL
1	A	499	VAL
1	A	504	LEU
1	A	510	VAL
1	B	82	ASN
1	B	113	PRO
1	B	116	LEU
1	B	174	VAL
1	B	213	VAL
1	B	214	GLU
1	B	230	ILE
1	B	232	GLU
1	B	290	GLN
1	B	328	ASP
1	B	411	VAL
1	B	438	VAL
1	B	499	VAL
1	B	504	LEU
1	B	510	VAL
1	C	82	ASN
1	C	113	PRO

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Mol	Chain	Res	Type
1	C	116	LEU
1	C	169	VAL
1	C	174	VAL
1	C	213	VAL
1	C	214	GLU
1	C	230	ILE
1	C	232	GLU
1	C	290	GLN
1	C	328	ASP
1	C	411	VAL
1	C	438	VAL
1	C	499	VAL
1	C	504	LEU
1	C	510	VAL
1	D	82	ASN
1	D	113	PRO
1	D	116	LEU
1	D	174	VAL
1	D	213	VAL
1	D	214	GLU
1	D	230	ILE
1	D	232	GLU
1	D	290	GLN
1	D	328	ASP
1	D	411	VAL
1	D	438	VAL
1	D	494	LEU
1	D	499	VAL
1	D	504	LEU
1	D	510	VAL
1	E	82	ASN
1	E	113	PRO
1	E	116	LEU
1	E	166	MET
1	E	174	VAL
1	E	213	VAL
1	E	214	GLU
1	E	230	ILE
1	E	232	GLU
1	E	290	GLN
1	E	328	ASP
1	E	411	VAL

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Mol	Chain	Res	Type
1	E	438	VAL
1	E	499	VAL
1	E	504	LEU
1	E	510	VAL
1	F	82	ASN
1	F	116	LEU
1	F	166	MET
1	F	174	VAL
1	F	213	VAL
1	F	214	GLU
1	F	230	ILE
1	F	232	GLU
1	F	290	GLN
1	F	328	ASP
1	F	411	VAL
1	F	438	VAL
1	F	499	VAL
1	F	504	LEU
1	F	510	VAL
1	G	82	ASN
1	G	116	LEU
1	G	166	MET
1	G	169	VAL
1	G	174	VAL
1	G	213	VAL
1	G	214	GLU
1	G	230	ILE
1	G	232	GLU
1	G	290	GLN
1	G	328	ASP
1	G	411	VAL
1	G	438	VAL
1	G	499	VAL
1	G	504	LEU
1	G	510	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	68	ASN
1	A	146	GLN

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Mol	Chain	Res	Type
1	A	194	GLN
1	A	319	GLN
1	A	348	GLN
1	A	352	GLN
1	A	436	GLN
1	A	437	ASN
1	A	453	GLN
1	B	10	ASN
1	B	37	ASN
1	B	68	ASN
1	B	146	GLN
1	B	194	GLN
1	B	319	GLN
1	B	348	GLN
1	B	352	GLN
1	B	437	ASN
1	B	453	GLN
1	C	10	ASN
1	C	68	ASN
1	C	146	GLN
1	C	184	GLN
1	C	194	GLN
1	C	319	GLN
1	C	348	GLN
1	C	352	GLN
1	C	437	ASN
1	C	453	GLN
1	D	10	ASN
1	D	68	ASN
1	D	146	GLN
1	D	194	GLN
1	D	319	GLN
1	D	348	GLN
1	D	352	GLN
1	D	437	ASN
1	D	453	GLN
1	E	10	ASN
1	E	68	ASN
1	E	146	GLN
1	E	194	GLN
1	E	319	GLN
1	E	348	GLN

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Mol	Chain	Res	Type
1	E	352	GLN
1	E	437	ASN
1	E	453	GLN
1	F	10	ASN
1	F	68	ASN
1	F	146	GLN
1	F	184	GLN
1	F	194	GLN
1	F	319	GLN
1	F	348	GLN
1	F	352	GLN
1	F	437	ASN
1	F	453	GLN
1	G	10	ASN
1	G	37	ASN
1	G	68	ASN
1	G	146	GLN
1	G	184	GLN
1	G	194	GLN
1	G	319	GLN
1	G	348	GLN
1	G	352	GLN
1	G	437	ASN
1	G	453	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.