



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:14 PM UTC

PDB ID : 1U0U / pdb_00001u0u
Title : An Aldol Switch Discovered in Stilbene Synthases Mediates Cyclization Specificity of Type III Polyketide Synthases: Pine stilbene synthase structure
Authors : Austin, M.B.; Bowman, M.E.; Ferrer, J.-L.; Schroder, J.; Noel, J.P.
Deposited on : 2004-07-14
Resolution : 2.11 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

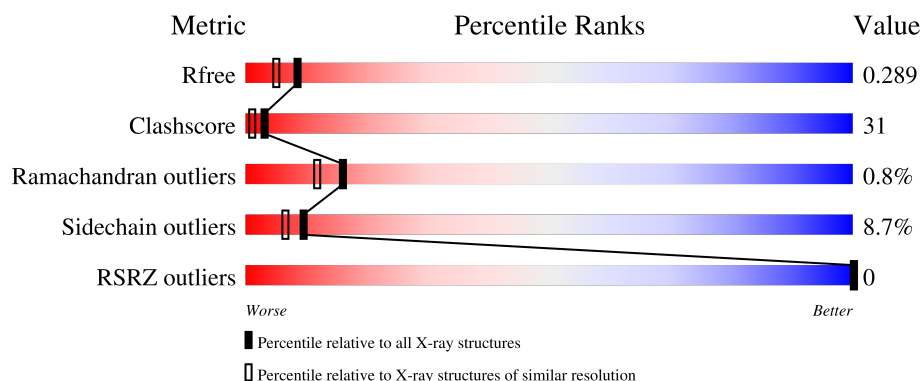
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	397	 62% 29% 7% •
1	B	397	 64% 29% 5% •
1	C	397	 60% 32% 6% •
1	D	397	 64% 29% • •
1	E	397	 63% 30% 5% •

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Mol	Chain	Length	Quality of chain
1	F	397	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (60%), yellow (32%), and orange (6%). The segments are labeled with their respective percentages: 60%, 32%, and 6%.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19745 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 Dihydropinosylvin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2979	1890	514	558	17			
1	B	389	Total	C	N	O	S	0	0	0
			2979	1890	514	558	17			
1	C	389	Total	C	N	O	S	0	0	0
			2979	1890	514	558	17			
1	D	389	Total	C	N	O	S	0	0	0
			2979	1890	514	558	17			
1	E	389	Total	C	N	O	S	0	0	0
			2979	1890	514	558	17			
1	F	389	Total	C	N	O	S	0	0	0
			2979	1890	514	558	17			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	cloning artifact	UNP Q02323
A	-2	SER	-	cloning artifact	UNP Q02323
A	-1	HIS	-	cloning artifact	UNP Q02323
A	0	GLY	-	cloning artifact	UNP Q02323
B	-3	GLY	-	cloning artifact	UNP Q02323
B	-2	SER	-	cloning artifact	UNP Q02323
B	-1	HIS	-	cloning artifact	UNP Q02323
B	0	GLY	-	cloning artifact	UNP Q02323
C	-3	GLY	-	cloning artifact	UNP Q02323
C	-2	SER	-	cloning artifact	UNP Q02323
C	-1	HIS	-	cloning artifact	UNP Q02323
C	0	GLY	-	cloning artifact	UNP Q02323
D	-3	GLY	-	cloning artifact	UNP Q02323
D	-2	SER	-	cloning artifact	UNP Q02323
D	-1	HIS	-	cloning artifact	UNP Q02323
D	0	GLY	-	cloning artifact	UNP Q02323
E	-3	GLY	-	cloning artifact	UNP Q02323

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	SER	-	cloning artifact	UNP Q02323
E	-1	HIS	-	cloning artifact	UNP Q02323
E	0	GLY	-	cloning artifact	UNP Q02323
F	-3	GLY	-	cloning artifact	UNP Q02323
F	-2	SER	-	cloning artifact	UNP Q02323
F	-1	HIS	-	cloning artifact	UNP Q02323
F	0	GLY	-	cloning artifact	UNP Q02323

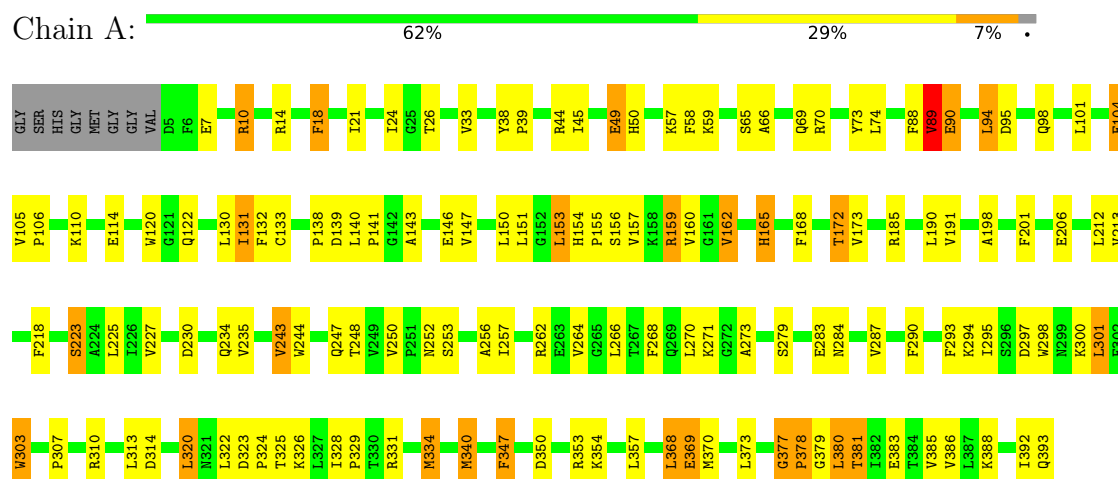
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	305	Total	O	0	0
			305	305		
2	B	342	Total	O	0	0
			342	342		
2	C	369	Total	O	0	0
			369	369		
2	D	309	Total	O	0	0
			309	309		
2	E	267	Total	O	0	0
			267	267		
2	F	279	Total	O	0	0
			279	279		

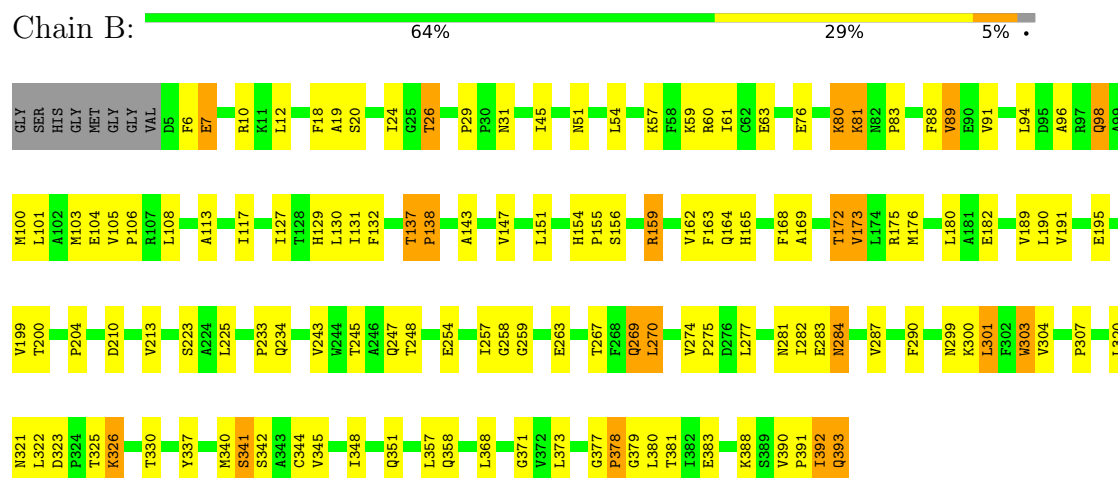
3 Residue-property plots [i](#)

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

• Molecule 1: Dihydropinosylvin synthase

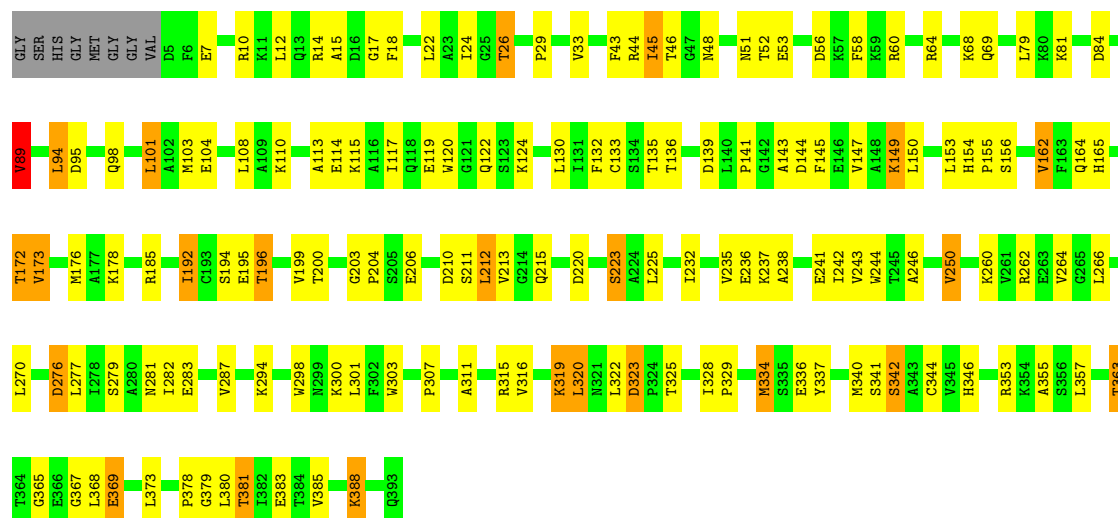


• Molecule 1: Dihydropinosylvin synthase



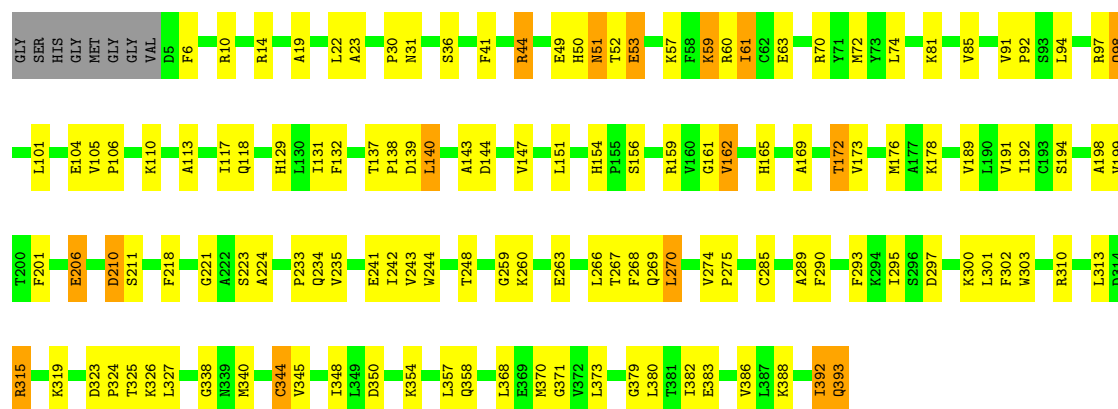
• Molecule 1: Dihydropinosylvin synthase





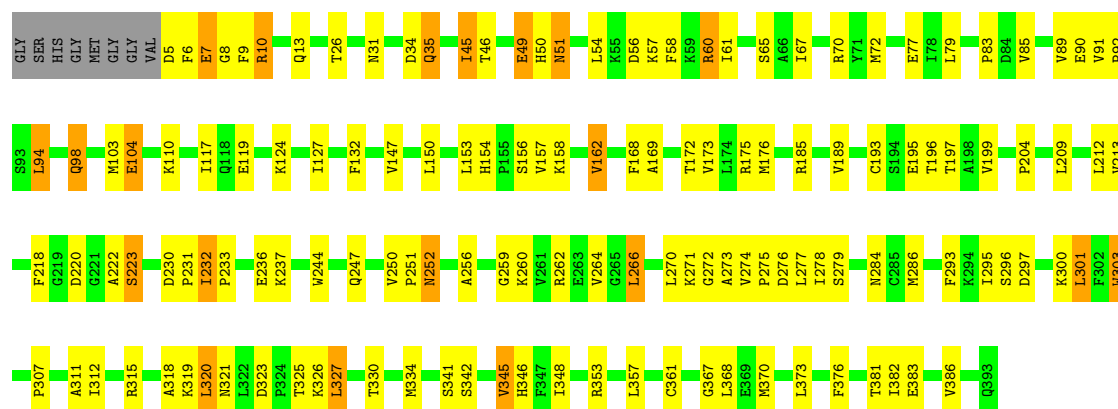
• Molecule 1: Dihydropinosylvic acid synthase

Chain D: 64% 29%



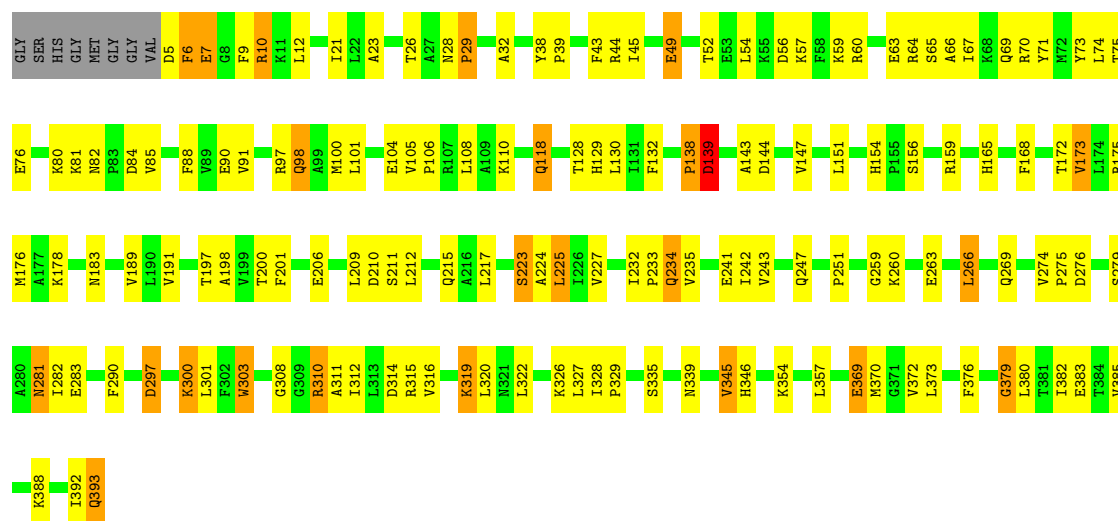
• Molecule 1: Dihydropinosylvic acid synthase

Chain E: 63% 30% 5%



• Molecule 1: Dihydropinosylvic acid synthase

Response	Percentage
Yes	60%
No	32%
Don't know	6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.22Å 361.29Å 57.32Å 90.00° 98.39° 90.00°	Depositor
Resolution (Å)	54.10 – 2.11 54.10 – 2.11	Depositor EDS
% Data completeness (in resolution range)	78.7 (54.10-2.11) 78.8 (54.10-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.289 0.225 , 0.289	Depositor DCC
R_{free} test set	5163 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.229 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19745	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	2/3039 (0.1%)	1.00	14/4115 (0.3%)
1	B	0.61	1/3039 (0.0%)	1.00	14/4115 (0.3%)
1	C	0.61	2/3039 (0.1%)	0.99	6/4115 (0.1%)
1	D	0.61	1/3039 (0.0%)	1.00	12/4115 (0.3%)
1	E	0.60	1/3039 (0.0%)	0.98	8/4115 (0.2%)
1	F	0.58	1/3039 (0.0%)	0.99	11/4115 (0.3%)
All	All	0.60	8/18234 (0.0%)	0.99	65/24690 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	223	SER	CB-OG	20.24	1.82	1.42
1	B	223	SER	CB-OG	18.77	1.79	1.42
1	A	223	SER	CB-OG	18.41	1.78	1.42
1	C	223	SER	CB-OG	18.33	1.78	1.42
1	D	223	SER	CB-OG	17.80	1.77	1.42
1	F	223	SER	CB-OG	17.68	1.77	1.42
1	C	334	MET	SD-CE	-6.38	1.63	1.79
1	A	334	MET	SD-CE	-5.00	1.67	1.79

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	165	HIS	N-CA-C	-10.84	99.57	113.12
1	F	243	VAL	N-CA-C	8.50	119.06	110.82
1	A	377	GLY	CA-C-N	7.80	129.59	119.84
1	A	377	GLY	C-N-CA	7.80	129.59	119.84
1	B	243	VAL	N-CA-C	7.61	118.53	111.45
1	A	235	VAL	N-CA-C	-7.55	105.77	112.12
1	F	6	PHE	N-CA-C	-7.51	103.03	111.14
1	F	29	PRO	N-CA-C	-7.36	103.41	110.47
1	F	138	PRO	N-CA-C	7.25	122.93	113.86
1	A	303	TRP	N-CA-C	7.16	121.08	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	243	VAL	N-CA-C	7.15	118.10	111.45
1	B	7	GLU	N-CA-C	-6.73	104.94	113.01
1	F	139	ASP	N-CA-C	6.67	116.79	108.19
1	D	192	ILE	N-CA-C	6.54	117.53	108.12
1	A	243	VAL	N-CA-C	6.51	117.14	110.82
1	B	326	LYS	N-CA-C	6.49	118.15	111.14
1	D	290	PHE	N-CA-C	6.40	121.37	113.50
1	E	8	GLY	N-CA-C	-6.33	104.88	113.37
1	A	165	HIS	N-CA-C	-6.31	104.29	112.68
1	B	303	TRP	N-CA-C	6.30	119.67	109.40
1	D	243	VAL	N-CA-C	6.30	118.26	111.58
1	A	138	PRO	N-CA-C	6.29	121.80	113.57
1	B	137	THR	CA-C-N	6.22	125.78	119.19
1	B	137	THR	C-N-CA	6.22	125.78	119.19
1	D	104	GLU	N-CA-C	6.16	117.99	111.28
1	D	303	TRP	N-CA-C	6.14	119.21	109.50
1	D	218	PHE	N-CA-C	6.13	119.23	110.10
1	B	322	LEU	N-CA-C	-6.05	101.97	110.50
1	F	217	LEU	N-CA-C	6.03	120.70	112.68
1	B	31	ASN	N-CA-C	6.01	118.25	108.63
1	F	104	GLU	N-CA-C	6.00	117.49	111.07
1	B	341	SER	CB-CA-C	-5.95	109.72	116.63
1	F	189	VAL	N-CA-C	5.92	117.10	108.58
1	A	114	GLU	N-CA-C	-5.89	104.86	111.28
1	D	235	VAL	N-CA-C	5.89	116.35	110.23
1	B	290	PHE	N-CA-C	5.81	120.65	113.50
1	E	346	HIS	N-CA-C	-5.77	105.07	111.36
1	A	218	PHE	N-CA-C	5.73	118.76	110.28
1	D	139	ASP	N-CA-C	5.69	115.92	108.07
1	C	104	GLU	N-CA-C	5.68	117.14	111.07
1	F	327	LEU	N-CA-C	5.67	119.28	112.93
1	A	104	GLU	N-CA-C	5.65	117.24	111.14
1	B	165	HIS	N-CA-C	-5.55	105.30	112.68
1	E	218	PHE	N-CA-C	5.47	118.16	110.23
1	E	303	TRP	N-CA-C	5.44	118.42	109.72
1	C	355	ALA	N-CA-C	-5.42	105.37	111.28
1	F	165	HIS	N-CA-C	-5.40	106.82	113.41
1	E	189	VAL	N-CA-C	5.39	116.35	108.58
1	E	104	GLU	N-CA-C	5.39	116.96	111.14
1	D	19	ALA	N-CA-C	-5.34	102.37	110.28
1	B	138	PRO	N-CA-C	5.29	120.50	113.57
1	C	342	SER	N-CA-C	5.26	117.76	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	HIS	N-CA-C	5.26	117.01	111.28
1	E	327	LEU	N-CA-C	5.17	119.54	112.88
1	B	104	GLU	N-CA-C	5.16	116.71	111.14
1	C	192	ILE	N-CA-C	5.15	116.14	108.46
1	C	264	VAL	N-CA-C	-5.15	107.45	112.29
1	D	138	PRO	N-CA-C	5.14	120.58	113.65
1	E	85	VAL	N-CA-C	-5.13	104.86	112.04
1	B	159	ARG	N-CA-C	5.12	118.16	109.76
1	A	340	MET	N-CA-C	-5.11	107.55	112.97
1	F	303	TRP	N-CA-C	5.08	117.84	109.72
1	A	347	PHE	N-CA-C	-5.05	105.78	111.28
1	A	279	SER	N-CA-C	5.03	116.45	111.07
1	D	344	CYS	N-CA-C	5.01	117.13	111.02

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	2979	0	2987	115	0
1	B	2979	0	2987	102	0
1	C	2979	0	2987	121	0
1	D	2979	0	2987	102	0
1	E	2979	0	2987	106	0
1	F	2979	0	2987	109	0
2	A	305	0	0	6	0
2	B	342	0	0	10	0
2	C	369	0	0	12	0
2	D	309	0	0	11	0
2	E	267	0	0	7	0
2	F	279	0	0	6	0
All	All	19745	0	17922	624	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 31.

All (624) 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:F:223:SER:CB	1:F:223:SER:OG	1.77	1.30
1:A:223:SER:CB	1:A:223:SER:OG	1.79	1.30
1:C:363:THR:HG23	1:C:365:GLY:H	1.19	1.08
1:D:173:VAL:HG11	1:D:191:VAL:HG13	1.36	1.03
1:F:97:ARG:HA	1:F:100:MET:HE2	1.41	0.98
1:B:162:VAL:HG21	1:B:176:MET:HE1	1.46	0.96
1:D:169:ALA:HA	1:D:172:THR:HG23	1.46	0.96
1:D:98:GLN:HA	1:D:98:GLN:HE21	1.27	0.95
1:C:206:GLU:HG2	2:C:535:HOH:O	1.68	0.94
1:A:381:THR:HG21	1:B:159:ARG:HH22	1.34	0.92
1:E:376:PHE:CD1	1:E:382:ILE:HD12	2.05	0.92
1:F:279:SER:OG	1:F:315:ARG:HB3	1.70	0.91
1:C:154:HIS:HD2	1:C:156:SER:H	1.16	0.90
1:F:297:ASP:HB2	1:F:300:LYS:HE3	1.52	0.90
1:F:10:ARG:HH12	1:F:183:ASN:ND2	1.69	0.90
1:F:10:ARG:HH12	1:F:183:ASN:HD21	0.97	0.89
1:A:297:ASP:HB3	1:A:300:LYS:HE2	1.55	0.89
1:B:7:GLU:HA	2:B:621:HOH:O	1.72	0.87
1:A:322:LEU:HB3	1:A:326:LYS:HG3	1.57	0.86
1:F:345:VAL:HG13	1:F:373:LEU:HD11	1.58	0.85
1:A:131:ILE:HG21	1:A:173:VAL:HG13	1.59	0.85
1:F:322:LEU:HB3	1:F:326:LYS:HG3	1.60	0.84
1:E:262:ARG:NH1	1:F:98:GLN:HG2	1.93	0.83
1:B:169:ALA:HA	1:B:172:THR:HG23	1.62	0.82
1:F:308:GLY:HA2	1:F:339:ASN:ND2	1.95	0.82
1:C:307:PRO:HB2	1:C:334:MET:HE3	1.62	0.81
1:B:98:GLN:HE21	1:B:98:GLN:HA	1.42	0.80
1:D:59:LYS:O	1:D:63:GLU:HG3	1.81	0.80
1:E:46:THR:HG21	1:E:204:PRO:HD2	1.64	0.80
1:E:35:GLN:HE22	1:E:70:ARG:HH21	1.28	0.79
1:E:323:ASP:HB2	1:E:325:THR:HG22	1.65	0.78
1:D:244:TRP:HB3	1:D:386:VAL:CG2	2.14	0.77
1:B:131:ILE:HD11	1:B:180:LEU:HD12	1.64	0.77
1:E:259:GLY:O	1:F:139:ASP:HB3	1.83	0.77
1:E:251:PRO:C	1:E:252:ASN:HD22	1.92	0.77
1:C:381:THR:HG21	1:D:159:ARG:HH22	1.48	0.76
1:C:103:MET:HG3	2:C:437:HOH:O	1.84	0.76
1:C:53:GLU:HB3	2:C:635:HOH:O	1.84	0.76
1:D:131:ILE:HG21	1:D:173:VAL:HG13	1.67	0.76
1:C:363:THR:HG22	1:C:367:GLY:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:ARG:HD3	2:E:563:HOH:O	1.86	0.76
1:A:151:LEU:HB3	1:A:153:LEU:HD13	1.67	0.75
1:A:244:TRP:HB3	1:A:386:VAL:HG11	1.67	0.75
1:B:108:LEU:HD12	2:B:631:HOH:O	1.86	0.75
1:C:369:GLU:CD	1:C:369:GLU:H	1.93	0.75
1:F:345:VAL:HG12	1:F:346:HIS:CD2	2.23	0.74
1:A:44:ARG:HA	1:A:49:GLU:OE1	1.88	0.74
1:A:105:VAL:HB	1:A:106:PRO:HD3	1.68	0.73
1:A:244:TRP:O	1:A:386:VAL:HG12	1.88	0.73
1:C:363:THR:HG22	1:C:367:GLY:H	1.52	0.73
1:E:295:ILE:CG2	1:E:301:LEU:HD21	2.18	0.73
1:E:247:GLN:HB2	1:E:383:GLU:OE2	1.88	0.73
1:C:135:THR:HG22	1:C:136:THR:HG23	1.70	0.73
1:D:110:LYS:HG3	1:D:151:LEU:HD23	1.71	0.72
1:F:328:ILE:HB	1:F:329:PRO:HD3	1.72	0.71
1:A:39:PRO:CB	1:A:59:LYS:HG2	2.20	0.71
1:A:328:ILE:HB	1:A:329:PRO:HD3	1.72	0.71
1:C:319:LYS:HE2	1:C:319:LYS:O	1.89	0.71
1:F:105:VAL:HB	1:F:106:PRO:HD3	1.73	0.71
1:C:89:VAL:HG13	1:C:89:VAL:O	1.89	0.71
1:F:251:PRO:HD2	1:F:281:ASN:HD21	1.55	0.71
1:A:392:ILE:O	1:A:393:GLN:HG2	1.91	0.70
1:F:379:GLY:HA3	1:F:380:LEU:C	2.16	0.70
1:F:197:THR:HA	1:F:200:THR:HG22	1.73	0.70
1:A:268:PHE:CZ	1:A:270:LEU:HB2	2.27	0.70
1:E:92:PRO:HB2	1:F:263:GLU:OE2	1.91	0.70
1:F:59:LYS:HG2	1:F:63:GLU:OE2	1.91	0.70
1:B:345:VAL:HG21	1:B:373:LEU:HD21	1.74	0.70
1:B:393:GLN:H	1:B:393:GLN:HE21	1.39	0.70
1:C:58:PHE:CD2	1:C:212:LEU:HD22	2.26	0.70
1:D:113:ALA:O	1:D:117:ILE:HG12	1.92	0.70
1:D:92:PRO:HB3	2:D:454:HOH:O	1.92	0.70
1:C:210:ASP:HB2	1:C:270:LEU:HD23	1.72	0.69
1:D:326:LYS:HE2	1:D:326:LYS:HA	1.73	0.69
1:A:89:VAL:HG22	1:A:264:VAL:HG11	1.75	0.69
1:B:88:PHE:CD2	1:B:89:VAL:HG22	2.27	0.69
1:D:154:HIS:CD2	1:D:156:SER:HB2	2.27	0.69
1:F:191:VAL:HB	1:F:225:LEU:CD1	2.20	0.69
1:E:54:LEU:HD21	1:E:204:PRO:HB2	1.74	0.69
1:C:363:THR:HG23	1:C:365:GLY:N	2.02	0.69
1:D:60:ARG:NH1	1:E:318:ALA:O	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:PHE:O	1:A:295:ILE:HG13	1.93	0.69
1:D:319:LYS:O	1:D:319:LYS:HD3	1.91	0.69
1:E:172:THR:HG22	1:E:175:ARG:HH21	1.57	0.69
1:A:10:ARG:HG2	1:B:18:PHE:CE2	2.28	0.69
1:D:105:VAL:HB	1:D:106:PRO:HD3	1.74	0.69
1:C:154:HIS:CD2	1:C:156:SER:H	2.05	0.68
1:F:376:PHE:CD1	1:F:382:ILE:HD12	2.29	0.68
1:A:307:PRO:HB2	1:A:334:MET:HG3	1.74	0.68
1:B:113:ALA:O	1:B:117:ILE:HG12	1.92	0.68
1:A:381:THR:HG21	1:B:159:ARG:NH2	2.06	0.68
1:C:232:ILE:HG23	1:C:235:VAL:HB	1.76	0.68
1:C:250:VAL:HG12	1:C:380:LEU:O	1.95	0.67
1:C:328:ILE:HB	1:C:329:PRO:HD3	1.76	0.67
1:D:268:PHE:CZ	1:D:270:LEU:HB2	2.30	0.67
1:C:323:ASP:OD2	1:C:325:THR:HG22	1.95	0.67
1:E:132:PHE:CE2	1:E:147:VAL:HG21	2.30	0.67
1:F:172:THR:HG22	1:F:383:GLU:OE2	1.94	0.67
1:B:98:GLN:HG3	1:B:138:PRO:CB	2.25	0.66
1:A:379:GLY:N	1:A:380:LEU:HA	2.10	0.66
1:C:117:ILE:HG21	1:C:124:LYS:HG2	1.76	0.66
1:E:5:ASP:HB2	2:E:557:HOH:O	1.95	0.66
1:A:268:PHE:HZ	1:A:270:LEU:HD22	1.60	0.66
1:F:376:PHE:HD1	1:F:382:ILE:HD12	1.59	0.66
1:F:312:ILE:O	1:F:316:VAL:HG23	1.96	0.66
1:C:110:LYS:O	1:C:114:GLU:HG2	1.95	0.66
1:A:33:VAL:HG22	1:A:70:ARG:O	1.95	0.65
1:B:29:PRO:HG3	1:B:108:LEU:HD11	1.79	0.65
1:A:162:VAL:HG23	1:A:165:HIS:CE1	2.31	0.65
1:E:244:TRP:HB3	1:E:386:VAL:HG11	1.79	0.65
1:D:268:PHE:HZ	1:D:270:LEU:HD12	1.62	0.65
1:D:268:PHE:CZ	1:D:270:LEU:HD12	2.31	0.65
1:B:113:ALA:HB3	1:B:151:LEU:HD21	1.79	0.64
1:A:262:ARG:NH1	1:B:98:GLN:HG2	2.12	0.64
1:C:68:LYS:HE2	2:C:455:HOH:O	1.97	0.64
1:E:300:LYS:C	1:E:368:LEU:HD23	2.23	0.64
1:F:379:GLY:N	1:F:380:LEU:HA	2.11	0.64
1:D:53:GLU:HG3	2:D:562:HOH:O	1.97	0.64
1:C:132:PHE:CE2	1:C:147:VAL:HG21	2.33	0.64
1:E:323:ASP:CB	1:E:325:THR:HG22	2.27	0.64
1:D:392:ILE:HD12	1:D:393:GLN:O	1.97	0.64
1:E:270:LEU:C	1:E:270:LEU:HD23	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:HIS:ND1	1:B:180:LEU:HD22	2.13	0.63
1:F:73:TYR:HE2	1:F:100:MET:HB3	1.63	0.63
1:F:128:THR:OG1	1:F:129:HIS:HD2	1.82	0.63
1:E:251:PRO:C	1:E:252:ASN:ND2	2.56	0.63
1:F:393:GLN:HA	1:F:393:GLN:HE21	1.63	0.62
1:A:257:ILE:HG22	1:A:378:PRO:HG3	1.81	0.62
1:B:274:VAL:HB	1:B:275:PRO:HD3	1.81	0.62
1:D:169:ALA:HA	1:D:172:THR:CG2	2.25	0.62
1:F:373:LEU:HB3	1:F:385:VAL:HB	1.82	0.62
1:F:98:GLN:HG3	1:F:138:PRO:HB3	1.81	0.62
1:F:369:GLU:CD	1:F:370:MET:HG3	2.24	0.62
1:B:57:LYS:O	1:B:61:ILE:HG13	2.00	0.62
1:C:18:PHE:CE1	1:D:6:PHE:HD2	2.05	0.62
1:F:154:HIS:CD2	1:F:156:SER:H	2.18	0.62
1:E:154:HIS:O	1:E:157:VAL:HG23	1.99	0.62
1:D:173:VAL:HG11	1:D:191:VAL:CG1	2.23	0.61
1:C:12:LEU:HD21	2:C:416:HOH:O	1.99	0.61
1:D:379:GLY:N	1:D:380:LEU:HA	2.15	0.61
1:B:199:VAL:HG13	1:B:200:THR:HG23	1.82	0.61
1:D:315:ARG:HH21	1:E:368:LEU:HD11	1.64	0.61
1:E:297:ASP:H	1:E:300:LYS:HE2	1.65	0.61
1:C:29:PRO:HG3	1:C:108:LEU:HD11	1.83	0.61
1:C:154:HIS:HD2	1:C:156:SER:N	1.93	0.61
1:C:266:LEU:C	1:C:266:LEU:HD23	2.25	0.61
1:B:195:GLU:HG3	1:B:341:SER:HB3	1.83	0.60
1:D:350:ASP:O	1:D:354:LYS:HG2	2.01	0.60
1:E:162:VAL:CG2	1:E:162:VAL:O	2.49	0.60
1:C:60:ARG:O	1:C:64:ARG:HG2	2.01	0.60
1:D:313:LEU:HD22	1:D:327:LEU:HD13	1.84	0.60
1:A:89:VAL:O	1:A:89:VAL:HG13	2.01	0.60
1:D:131:ILE:CG2	1:D:173:VAL:HG13	2.32	0.60
1:D:244:TRP:HB3	1:D:386:VAL:HG22	1.82	0.60
1:D:98:GLN:HE21	1:D:98:GLN:CA	2.04	0.59
1:D:172:THR:HG22	1:D:383:GLU:OE2	2.02	0.59
1:F:44:ARG:HA	1:F:49:GLU:HG2	1.84	0.59
1:B:154:HIS:ND1	1:B:155:PRO:HD2	2.17	0.59
1:C:241:GLU:OE1	1:C:388:LYS:HE2	2.02	0.59
1:D:57:LYS:O	1:D:61:ILE:HD13	2.03	0.59
1:E:315:ARG:NH1	1:E:315:ARG:HB3	2.17	0.59
1:B:358:GLN:O	1:B:358:GLN:HG2	2.01	0.59
1:B:117:ILE:CD1	1:B:127:ILE:HD11	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:HIS:CD2	1:B:156:SER:H	2.21	0.59
1:D:36:SER:HA	2:D:479:HOH:O	2.02	0.59
1:F:154:HIS:CD2	1:F:156:SER:HB2	2.38	0.59
1:E:193:CYS:O	1:E:222:ALA:HA	2.03	0.59
1:E:293:PHE:HB3	1:E:370:MET:HE1	1.84	0.59
1:F:74:LEU:HD11	1:F:198:ALA:HA	1.84	0.58
1:F:308:GLY:HA2	1:F:339:ASN:HD22	1.64	0.58
1:E:7:GLU:HA	1:E:10:ARG:HB2	1.83	0.58
1:E:117:ILE:HD12	1:E:127:ILE:HD11	1.85	0.58
1:D:358:GLN:O	1:D:358:GLN:HG2	2.03	0.58
1:E:278:ILE:C	1:E:278:ILE:HD12	2.28	0.58
1:C:15:ALA:HB2	1:C:185:ARG:HA	1.86	0.58
1:C:165:HIS:CE1	1:D:161:GLY:H	2.22	0.58
1:F:310:ARG:HG2	1:F:314:ASP:OD2	2.03	0.58
1:D:30:PRO:HB2	2:D:422:HOH:O	2.04	0.58
1:E:279:SER:O	1:E:319:LYS:HG3	2.04	0.58
1:E:368:LEU:N	1:E:368:LEU:HD12	2.19	0.58
1:F:38:TYR:N	1:F:39:PRO:HD2	2.19	0.58
1:A:89:VAL:CG2	1:A:264:VAL:HG11	2.34	0.57
1:B:172:THR:HB	1:B:175:ARG:NH2	2.18	0.57
1:F:143:ALA:O	1:F:147:VAL:HG23	2.04	0.57
1:A:256:ALA:HB3	1:A:380:LEU:CD1	2.33	0.57
1:B:132:PHE:HE2	1:B:147:VAL:HG21	1.68	0.57
1:E:311:ALA:HB3	2:E:405:HOH:O	2.04	0.57
1:A:94:LEU:HG	1:A:262:ARG:O	2.04	0.57
1:C:173:VAL:HA	1:C:176:MET:HE2	1.86	0.57
1:F:154:HIS:HD2	1:F:156:SER:HB2	1.68	0.57
1:F:173:VAL:HG13	1:F:191:VAL:HG11	1.85	0.57
1:B:143:ALA:O	1:B:147:VAL:HG23	2.04	0.57
1:A:323:ASP:O	1:A:325:THR:N	2.38	0.57
1:D:340:MET:N	1:D:344:CYS:SG	2.76	0.57
1:F:282:ILE:HG12	1:F:320:LEU:HD11	1.87	0.57
1:A:252:ASN:HB2	2:A:633:HOH:O	2.04	0.57
1:B:393:GLN:NE2	1:B:393:GLN:N	2.53	0.57
1:D:132:PHE:CE1	1:D:143:ALA:HB3	2.39	0.57
1:E:91:VAL:CG2	1:E:92:PRO:HD2	2.34	0.57
1:B:299:ASN:HA	1:B:326:LYS:HE3	1.87	0.56
1:C:124:LYS:HD3	2:C:627:HOH:O	2.04	0.56
1:E:244:TRP:H	1:E:386:VAL:CG1	2.18	0.56
1:B:321:ASN:HA	2:B:521:HOH:O	2.06	0.56
1:D:324:PRO:HB2	2:D:673:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ILE:CG2	1:C:235:VAL:HB	2.36	0.56
1:D:233:PRO:O	1:D:234:GLN:HB3	2.04	0.56
1:E:117:ILE:HG21	1:E:124:LYS:HG3	1.88	0.56
1:F:172:THR:O	1:F:176:MET:HG3	2.06	0.56
1:B:127:ILE:HD13	1:B:190:LEU:HD22	1.87	0.56
1:C:98:GLN:NE2	1:C:98:GLN:HA	2.20	0.56
1:B:105:VAL:HB	1:B:106:PRO:HD3	1.88	0.56
1:C:132:PHE:CE1	1:C:143:ALA:HB3	2.41	0.56
1:F:73:TYR:CE2	1:F:100:MET:HB3	2.40	0.56
1:E:158:LYS:HB3	1:F:175:ARG:NH1	2.21	0.55
1:F:269:GLN:NE2	2:F:613:HOH:O	2.39	0.55
1:B:341:SER:OG	1:B:342:SER:N	2.40	0.55
1:D:59:LYS:O	1:D:59:LYS:HD3	2.06	0.55
1:E:110:LYS:HD2	1:E:150:LEU:HB3	1.89	0.55
1:C:172:THR:HB	1:C:383:GLU:OE2	2.07	0.55
1:F:43:PHE:CZ	1:F:54:LEU:HB3	2.42	0.55
1:B:258:GLY:O	1:B:269:GLN:HG2	2.07	0.54
1:C:241:GLU:HB2	1:C:388:LYS:HB3	1.90	0.54
1:C:379:GLY:N	1:C:380:LEU:HA	2.22	0.54
1:F:21:ILE:HD13	1:F:227:VAL:HG22	1.88	0.54
1:C:155:PRO:O	1:D:248:THR:HA	2.06	0.54
1:E:237:LYS:HE2	2:E:525:HOH:O	2.06	0.54
1:A:325:THR:O	1:A:328:ILE:HG12	2.06	0.54
1:A:350:ASP:O	1:A:354:LYS:HG2	2.08	0.54
1:B:282:ILE:HG23	1:B:320:LEU:HD21	1.87	0.54
1:F:345:VAL:CG1	1:F:373:LEU:HD11	2.32	0.54
1:A:139:ASP:C	1:A:140:LEU:HD12	2.33	0.54
1:E:256:ALA:HA	1:E:271:LYS:HB2	1.90	0.54
1:E:272:GLY:O	1:E:275:PRO:HD2	2.07	0.54
1:A:21:ILE:HD13	1:A:227:VAL:HG22	1.89	0.54
1:A:297:ASP:OD2	1:A:300:LYS:HG3	2.07	0.54
1:B:45:ILE:HD13	1:B:76:GLU:HG3	1.88	0.54
1:B:392:ILE:O	1:B:392:ILE:HG13	2.06	0.54
1:A:44:ARG:CA	1:A:49:GLU:OE1	2.55	0.54
1:C:210:ASP:OD1	1:C:211:SER:N	2.40	0.54
1:C:307:PRO:CB	1:C:334:MET:HE3	2.34	0.54
1:D:50:HIS:ND1	1:D:51:ASN:N	2.55	0.54
1:E:57:LYS:HZ1	1:E:209:LEU:HD13	1.73	0.54
1:A:141:PRO:HD3	1:B:378:PRO:HB3	1.88	0.54
1:C:14:ARG:C	1:C:185:ARG:HB2	2.33	0.54
1:E:297:ASP:N	1:E:300:LYS:HE2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASP:C	1:A:325:THR:H	2.16	0.54
1:A:350:ASP:O	1:A:353:ARG:HG2	2.08	0.54
1:B:26:THR:HG23	2:B:573:HOH:O	2.08	0.54
1:B:368:LEU:N	1:B:368:LEU:HD22	2.23	0.54
1:A:295:ILE:HD11	1:A:370:MET:HE3	1.90	0.53
1:E:65:SER:C	1:E:67:ILE:H	2.16	0.53
1:A:139:ASP:HB3	1:B:259:GLY:O	2.08	0.53
1:B:304:VAL:HG12	1:B:345:VAL:HG23	1.91	0.53
1:C:120:TRP:CE2	1:C:122:GLN:HB2	2.43	0.53
1:E:381:THR:C	1:E:382:ILE:HD13	2.34	0.53
1:B:233:PRO:O	1:B:234:GLN:CG	2.56	0.53
1:B:277:LEU:O	1:B:281:ASN:ND2	2.35	0.53
1:B:390:VAL:HG13	1:B:391:PRO:HD2	1.90	0.53
1:E:162:VAL:O	1:E:162:VAL:HG22	2.09	0.53
1:A:156:SER:OG	1:B:248:THR:HG22	2.08	0.53
1:D:310:ARG:HG2	1:D:310:ARG:NH1	2.21	0.53
1:B:393:GLN:HE21	1:B:393:GLN:N	2.07	0.53
1:C:336:GLU:HB2	2:C:430:HOH:O	2.08	0.53
1:A:284:ASN:O	1:A:284:ASN:ND2	2.42	0.53
1:A:369:GLU:N	1:A:369:GLU:OE1	2.37	0.53
1:D:206:GLU:HG3	2:D:642:HOH:O	2.09	0.53
1:E:46:THR:HG22	1:E:46:THR:O	2.07	0.53
1:A:248:THR:O	1:A:381:THR:HA	2.09	0.53
1:F:232:ILE:HB	1:F:235:VAL:HB	1.90	0.53
1:A:162:VAL:HG23	1:A:165:HIS:ND1	2.25	0.52
1:F:241:GLU:HB2	1:F:388:LYS:HB3	1.89	0.52
1:C:363:THR:CG2	1:C:365:GLY:H	2.08	0.52
1:E:57:LYS:HZ3	1:E:209:LEU:HD13	1.74	0.52
1:D:178:LYS:HD2	1:D:242:ILE:HG22	1.91	0.52
1:C:164:GLN:C	1:D:140:LEU:HD13	2.32	0.52
1:B:307:PRO:HD2	1:B:344:CYS:HB3	1.90	0.52
1:F:81:LYS:HG3	1:F:81:LYS:O	2.09	0.52
1:A:378:PRO:O	1:A:381:THR:HG23	2.10	0.52
1:C:378:PRO:O	1:C:381:THR:HG23	2.09	0.52
1:E:323:ASP:HB2	1:E:325:THR:CG2	2.39	0.52
1:E:98:GLN:HA	1:E:98:GLN:NE2	2.14	0.52
1:F:21:ILE:HD11	1:F:242:ILE:HD11	1.91	0.52
1:F:224:ALA:C	1:F:225:LEU:HG	2.34	0.52
1:F:266:LEU:C	1:F:266:LEU:HD13	2.35	0.52
1:A:110:LYS:HE3	2:A:696:HOH:O	2.10	0.51
1:B:270:LEU:C	1:B:270:LEU:HD23	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:VAL:O	1:C:320:LEU:HD13	2.10	0.51
1:D:91:VAL:HG13	1:D:92:PRO:HD2	1.92	0.51
1:D:110:LYS:HA	1:D:151:LEU:HD21	1.92	0.51
1:A:293:PHE:O	1:A:294:LYS:HG3	2.10	0.51
1:B:379:GLY:HA3	1:B:381:THR:N	2.26	0.51
1:C:44:ARG:HD3	2:C:402:HOH:O	2.10	0.51
1:A:313:LEU:HD11	1:A:334:MET:HE3	1.92	0.51
1:D:300:LYS:HG2	2:D:565:HOH:O	2.08	0.51
1:A:58:PHE:CD2	1:A:212:LEU:HD22	2.45	0.51
1:B:24:ILE:HG12	1:B:225:LEU:CD2	2.40	0.51
1:D:129:HIS:HB2	1:D:189:VAL:HG13	1.93	0.51
1:B:259:GLY:HA2	1:B:267:THR:O	2.11	0.51
1:D:260:LYS:HB2	1:D:267:THR:OG1	2.10	0.51
1:F:392:ILE:O	1:F:392:ILE:HG13	2.10	0.51
1:C:232:ILE:HG22	1:C:236:GLU:HG3	1.92	0.51
1:D:210:ASP:CG	1:D:211:SER:N	2.68	0.51
1:F:45:ILE:HD12	2:F:459:HOH:O	2.11	0.51
1:C:94:LEU:HG	1:C:262:ARG:O	2.11	0.51
1:B:6:PHE:HE1	2:B:557:HOH:O	1.94	0.51
1:C:89:VAL:O	1:C:89:VAL:CG1	2.57	0.50
1:F:206:GLU:OE2	1:F:206:GLU:HA	2.11	0.50
1:A:250:VAL:HG23	1:A:253:SER:OG	2.11	0.50
1:E:119:GLU:CD	1:E:353:ARG:HH22	2.19	0.50
1:A:172:THR:HG22	1:A:383:GLU:OE2	2.11	0.50
1:B:162:VAL:CG2	1:B:176:MET:HE1	2.32	0.50
1:B:210:ASP:O	1:B:213:VAL:HB	2.12	0.50
1:B:392:ILE:HA	2:B:400:HOH:O	2.12	0.50
1:C:14:ARG:HD2	1:D:14:ARG:NH1	2.27	0.50
1:E:319:LYS:O	1:E:319:LYS:HD3	2.11	0.50
1:B:300:LYS:C	1:B:301:LEU:HD12	2.37	0.50
1:D:248:THR:HG22	1:D:382:ILE:HB	1.94	0.50
1:E:199:VAL:HG22	1:E:266:LEU:HB2	1.93	0.50
1:F:311:ALA:O	1:F:315:ARG:HB2	2.11	0.50
1:D:210:ASP:OD1	1:D:270:LEU:N	2.43	0.50
1:A:58:PHE:HD2	1:A:212:LEU:HD22	1.77	0.50
1:C:133:CYS:HB2	1:C:162:VAL:HG13	1.94	0.50
1:A:252:ASN:OD1	1:A:252:ASN:O	2.30	0.50
1:D:297:ASP:N	2:D:567:HOH:O	2.42	0.50
1:F:29:PRO:CD	1:F:108:LEU:HD11	2.33	0.50
1:F:75:THR:HB	2:F:419:HOH:O	2.12	0.50
1:C:369:GLU:CD	1:C:369:GLU:N	2.68	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:PHE:O	1:E:9:PHE:HB3	2.12	0.49
1:A:143:ALA:O	1:A:147:VAL:HG23	2.12	0.49
1:A:173:VAL:HG11	1:A:191:VAL:CG1	2.34	0.49
1:D:81:LYS:NZ	1:D:81:LYS:HB3	2.27	0.49
1:E:169:ALA:HB3	1:E:342:SER:CB	2.35	0.49
1:E:172:THR:C	1:E:176:MET:HE3	2.38	0.49
1:A:323:ASP:C	1:A:325:THR:N	2.70	0.49
1:F:100:MET:HE3	1:F:198:ALA:HB1	1.95	0.49
1:A:284:ASN:C	1:A:284:ASN:HD22	2.20	0.49
1:F:84:ASP:OD1	1:F:91:VAL:HG21	2.13	0.49
1:A:159:ARG:HG3	1:B:247:GLN:OE1	2.13	0.49
1:B:258:GLY:C	1:B:269:GLN:HG2	2.38	0.49
1:D:323:ASP:OD1	1:D:325:THR:HB	2.13	0.49
1:B:12:LEU:HD23	1:B:12:LEU:O	2.13	0.49
1:E:230:ASP:N	1:E:231:PRO:HD3	2.28	0.49
1:B:51:ASN:HD22	1:B:54:LEU:HD12	1.78	0.48
1:C:101:LEU:HD22	1:C:199:VAL:HB	1.95	0.48
1:C:244:TRP:CH2	1:C:246:ALA:HB2	2.48	0.48
1:C:337:TYR:CB	1:C:340:MET:HE2	2.43	0.48
1:F:274:VAL:HB	1:F:275:PRO:HD3	1.93	0.48
1:B:301:LEU:HB3	1:B:371:GLY:HA2	1.94	0.48
1:C:95:ASP:OD2	1:D:263:GLU:HG3	2.12	0.48
1:C:199:VAL:O	1:C:199:VAL:HG22	2.12	0.48
1:F:191:VAL:O	1:F:224:ALA:HA	2.12	0.48
1:E:31:ASN:HB3	1:E:72:MET:O	2.14	0.48
1:A:131:ILE:HD13	1:A:160:VAL:HG11	1.96	0.48
1:C:232:ILE:CG2	1:C:236:GLU:HG3	2.43	0.48
1:C:298:TRP:HB3	1:C:303:TRP:HZ2	1.78	0.48
1:C:110:LYS:O	1:C:110:LYS:HD2	2.14	0.48
1:D:173:VAL:CG1	1:D:191:VAL:CG1	2.89	0.48
1:A:368:LEU:CD1	1:A:368:LEU:N	2.76	0.48
1:C:24:ILE:HG23	1:C:225:LEU:HD23	1.95	0.48
1:C:311:ALA:HB3	2:C:664:HOH:O	2.13	0.48
1:A:24:ILE:HG12	1:A:225:LEU:HD22	1.96	0.48
1:A:373:LEU:HB3	1:A:385:VAL:HB	1.96	0.48
1:C:260:LYS:HD3	1:C:262:ARG:NH2	2.28	0.48
1:E:320:LEU:O	1:E:321:ASN:C	2.56	0.48
1:F:5:ASP:CG	1:F:6:PHE:N	2.72	0.48
1:F:282:ILE:HG23	1:F:283:GLU:N	2.29	0.47
1:A:133:CYS:HB2	1:A:162:VAL:CG1	2.44	0.47
1:E:94:LEU:HD22	1:E:98:GLN:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:ILE:HG23	1:E:236:GLU:HG3	1.96	0.47
1:C:45:ILE:CG2	1:C:79:LEU:HD13	2.40	0.47
1:D:172:THR:O	1:D:176:MET:HG3	2.13	0.47
1:F:393:GLN:HE21	1:F:393:GLN:N	2.12	0.47
1:A:7:GLU:HG3	2:A:684:HOH:O	2.13	0.47
1:A:14:ARG:C	1:A:185:ARG:HB2	2.40	0.47
1:C:43:PHE:HE1	1:C:58:PHE:CD1	2.32	0.47
1:C:250:VAL:HG23	1:C:281:ASN:ND2	2.29	0.47
1:D:52:THR:HG21	2:D:558:HOH:O	2.13	0.47
1:F:290:PHE:HZ	1:F:372:VAL:HB	1.79	0.47
1:A:140:LEU:HD11	1:B:164:GLN:HG2	1.96	0.47
1:A:303:TRP:CH2	1:A:320:LEU:HD23	2.50	0.47
1:B:129:HIS:HB2	1:B:189:VAL:HG22	1.96	0.47
1:C:22:LEU:HD23	1:C:238:ALA:HA	1.95	0.47
1:C:149:LYS:HD3	1:C:149:LYS:C	2.40	0.47
1:F:168:PHE:CD1	1:F:168:PHE:C	2.92	0.47
1:C:282:ILE:CG2	1:C:283:GLU:N	2.78	0.47
1:D:132:PHE:HB3	1:D:144:ASP:HB3	1.96	0.47
1:E:326:LYS:C	1:E:327:LEU:HD12	2.40	0.47
1:F:7:GLU:OE1	1:F:7:GLU:HA	2.14	0.47
1:C:232:ILE:HG22	1:C:236:GLU:CG	2.45	0.47
1:A:154:HIS:O	1:A:157:VAL:HG23	2.15	0.47
1:A:314:ASP:OD1	1:A:331:ARG:NH2	2.46	0.47
1:F:44:ARG:HD3	2:F:573:HOH:O	2.15	0.47
1:B:169:ALA:HA	1:B:172:THR:CG2	2.40	0.47
1:D:154:HIS:HD2	1:D:156:SER:HB2	1.77	0.47
1:C:196:THR:HA	1:C:220:ASP:CG	2.40	0.46
1:F:5:ASP:O	1:F:9:PHE:N	2.44	0.46
1:F:64:ARG:HD3	2:F:509:HOH:O	2.15	0.46
1:A:98:GLN:HE21	1:A:98:GLN:HA	1.80	0.46
1:E:195:GLU:HG3	1:E:341:SER:HB3	1.97	0.46
1:E:260:LYS:O	1:E:266:LEU:HD23	2.15	0.46
1:B:117:ILE:HD12	1:B:127:ILE:HD11	1.98	0.46
1:D:293:PHE:CG	1:D:370:MET:HE1	2.50	0.46
1:F:32:ALA:HB2	1:F:71:TYR:CE2	2.50	0.46
1:F:233:PRO:O	1:F:234:GLN:CG	2.63	0.46
1:C:46:THR:O	1:C:46:THR:CG2	2.63	0.46
1:E:83:PRO:HG3	2:E:480:HOH:O	2.15	0.46
1:A:154:HIS:CD2	1:A:156:SER:H	2.33	0.46
1:A:381:THR:CG2	1:B:159:ARG:HH22	2.18	0.46
1:D:221:GLY:HA3	1:D:340:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:CYS:SG	1:D:382:ILE:HG21	2.55	0.46
1:A:38:TYR:N	1:A:39:PRO:CD	2.79	0.46
1:C:178:LYS:HD2	1:C:242:ILE:HG22	1.97	0.46
1:D:154:HIS:CD2	1:D:156:SER:H	2.33	0.46
1:F:209:LEU:O	1:F:212:LEU:HB3	2.14	0.46
1:F:251:PRO:HD2	1:F:281:ASN:ND2	2.25	0.46
1:C:132:PHE:CD2	1:C:147:VAL:HG21	2.51	0.46
1:F:147:VAL:HG12	1:F:151:LEU:HD12	1.98	0.46
1:B:337:TYR:HB3	1:B:340:MET:HE2	1.97	0.46
1:D:31:ASN:HB3	1:D:72:MET:O	2.16	0.46
1:B:54:LEU:HD23	1:B:57:LYS:HD3	1.98	0.46
1:B:98:GLN:HA	1:B:98:GLN:NE2	2.18	0.46
1:B:351:GLN:HA	1:B:351:GLN:NE2	2.30	0.46
1:C:320:LEU:CD1	1:C:320:LEU:N	2.77	0.46
1:B:80:LYS:HE3	2:B:552:HOH:O	2.15	0.46
1:E:61:ILE:HD13	1:E:213:VAL:HG22	1.98	0.46
1:F:259:GLY:C	1:F:260:LYS:HG3	2.41	0.46
1:D:113:ALA:HA	1:D:224:ALA:CB	2.45	0.45
1:A:300:LYS:C	1:A:301:LEU:HD12	2.41	0.45
1:B:323:ASP:OD1	1:B:325:THR:N	2.38	0.45
1:D:60:ARG:HH12	1:E:318:ALA:CA	2.29	0.45
1:E:357:LEU:C	1:E:357:LEU:HD13	2.42	0.45
1:B:162:VAL:HG21	1:B:176:MET:CE	2.33	0.45
1:B:303:TRP:HD1	1:B:326:LYS:HD2	1.81	0.45
1:C:46:THR:HG21	1:C:203:GLY:HA2	1.98	0.45
1:D:97:ARG:NH2	1:D:201:PHE:O	2.49	0.45
1:A:65:SER:O	1:A:66:ALA:HB3	2.15	0.45
1:A:130:LEU:HD12	1:A:190:LEU:O	2.17	0.45
1:F:98:GLN:HE21	1:F:98:GLN:HA	1.81	0.45
1:C:94:LEU:HD22	1:C:98:GLN:HG2	1.98	0.45
1:C:132:PHE:HB3	1:C:144:ASP:HB3	1.99	0.45
1:C:141:PRO:HA	2:D:468:HOH:O	2.16	0.45
1:A:206:GLU:OE1	1:A:206:GLU:N	2.47	0.45
1:B:304:VAL:HG12	1:B:345:VAL:CG2	2.46	0.45
1:C:58:PHE:HD2	1:C:212:LEU:HD22	1.77	0.45
1:C:341:SER:OG	1:C:342:SER:N	2.50	0.45
1:E:345:VAL:HB	1:E:373:LEU:HD11	1.99	0.45
1:F:266:LEU:C	1:F:266:LEU:CD1	2.90	0.45
1:A:268:PHE:CZ	1:A:270:LEU:HD22	2.46	0.45
1:A:307:PRO:HB2	1:A:334:MET:CG	2.46	0.45
1:C:26:THR:O	1:C:115:LYS:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LYS:HB3	1:D:81:LYS:HZ3	1.80	0.45
1:D:81:LYS:NZ	1:D:81:LYS:CB	2.80	0.45
1:D:97:ARG:NH1	1:D:201:PHE:O	2.49	0.45
1:D:326:LYS:HE2	1:D:326:LYS:N	2.31	0.44
1:F:303:TRP:CH2	1:F:320:LEU:HD13	2.52	0.44
1:C:250:VAL:CG2	1:C:281:ASN:ND2	2.80	0.44
1:D:345:VAL:HA	1:D:348:ILE:HD12	1.99	0.44
1:B:96:ALA:O	1:B:100:MET:HE3	2.16	0.44
1:C:119:GLU:OE1	1:C:353:ARG:NH2	2.34	0.44
1:E:45:ILE:HG21	1:E:79:LEU:HD13	2.00	0.44
1:E:168:PHE:CD1	1:E:168:PHE:C	2.95	0.44
1:F:65:SER:O	1:F:66:ALA:HB3	2.17	0.44
1:A:120:TRP:CD2	1:A:122:GLN:HB2	2.53	0.44
1:C:210:ASP:O	1:C:213:VAL:HB	2.18	0.44
1:D:392:ILE:O	1:D:392:ILE:HG13	2.18	0.44
1:E:297:ASP:HB3	1:E:300:LYS:HG3	2.00	0.44
1:F:132:PHE:HB3	1:F:144:ASP:HB3	1.99	0.44
1:A:273:ALA:HA	2:A:498:HOH:O	2.17	0.44
1:D:70:ARG:HG2	1:D:338:GLY:HA3	1.99	0.44
1:B:168:PHE:CE1	1:B:172:THR:HG21	2.52	0.44
1:B:173:VAL:CG1	1:B:191:VAL:HG11	2.46	0.44
1:E:49:GLU:C	1:E:51:ASN:N	2.75	0.44
1:A:212:LEU:O	1:A:213:VAL:C	2.60	0.44
1:A:310:ARG:HG2	1:A:314:ASP:OD2	2.16	0.44
1:D:315:ARG:HH21	1:E:368:LEU:CD1	2.29	0.44
1:E:89:VAL:CG2	1:E:264:VAL:HG11	2.47	0.44
1:A:256:ALA:HA	1:A:271:LYS:HB2	2.00	0.44
1:A:303:TRP:HH2	1:A:320:LEU:HD23	1.82	0.44
1:C:211:SER:O	1:C:215:GLN:HG2	2.18	0.44
1:F:154:HIS:HD2	1:F:156:SER:H	1.63	0.44
1:A:247:GLN:HB2	1:A:383:GLU:OE1	2.18	0.43
1:B:284:ASN:O	1:B:287:VAL:HG22	2.17	0.43
1:C:279:SER:OG	1:C:315:ARG:HG3	2.17	0.43
1:E:77:GLU:OE1	1:E:77:GLU:N	2.45	0.43
1:C:162:VAL:HG23	1:C:165:HIS:CE1	2.53	0.43
1:D:101:LEU:HD21	1:D:199:VAL:HB	1.99	0.43
1:F:56:ASP:OD1	1:F:60:ARG:NH2	2.51	0.43
1:A:303:TRP:CD1	1:A:326:LYS:HD3	2.53	0.43
1:D:325:THR:O	1:D:326:LYS:C	2.61	0.43
1:E:110:LYS:CD	1:E:150:LEU:HB3	2.48	0.43
1:C:139:ASP:HB3	1:D:259:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:ALA:O	1:D:147:VAL:HG23	2.18	0.43
1:B:159:ARG:NH2	2:B:464:HOH:O	2.50	0.43
1:E:296:SER:N	1:E:300:LYS:HZ1	1.95	0.43
1:A:74:LEU:HD11	1:A:198:ALA:HA	2.00	0.43
1:C:323:ASP:OD2	1:C:325:THR:CG2	2.66	0.43
1:E:295:ILE:HG23	1:E:300:LYS:HE3	2.01	0.43
1:F:132:PHE:CD2	1:F:147:VAL:HG21	2.53	0.43
1:F:393:GLN:CA	1:F:393:GLN:NE2	2.78	0.43
1:A:110:LYS:HD2	1:A:150:LEU:HD23	2.01	0.43
1:E:65:SER:C	1:E:67:ILE:N	2.77	0.43
1:F:23:ALA:O	1:F:225:LEU:HB3	2.18	0.43
1:C:210:ASP:HB2	1:C:270:LEU:CD2	2.47	0.43
1:C:381:THR:HG21	1:D:159:ARG:NH2	2.27	0.43
1:D:22:LEU:O	1:D:23:ALA:HB2	2.17	0.43
1:E:286:MET:HE2	1:E:303:TRP:CZ2	2.54	0.43
1:B:54:LEU:HD13	1:B:204:PRO:HB2	2.01	0.43
1:A:95:ASP:OD2	1:B:263:GLU:HG3	2.18	0.43
1:B:81:LYS:C	1:B:83:PRO:HD3	2.44	0.43
1:F:82:ASN:HB3	1:F:85:VAL:HG23	2.01	0.43
1:A:132:PHE:O	1:A:162:VAL:HG12	2.19	0.42
1:C:114:GLU:HA	1:C:114:GLU:OE1	2.19	0.42
1:C:276:ASP:CG	1:C:277:LEU:N	2.77	0.42
1:E:232:ILE:HD12	1:E:233:PRO:CD	2.49	0.42
1:E:273:ALA:O	1:E:277:LEU:HG	2.19	0.42
1:E:311:ALA:O	1:E:312:ILE:C	2.62	0.42
1:E:330:THR:HA	1:E:348:ILE:HD13	2.01	0.42
1:C:319:LYS:C	1:C:320:LEU:HD12	2.45	0.42
1:D:260:LYS:HB2	1:D:267:THR:HG1	1.84	0.42
1:A:250:VAL:HG23	1:A:253:SER:CB	2.49	0.42
1:B:257:ILE:O	1:B:378:PRO:HA	2.18	0.42
1:C:237:LYS:HE2	2:C:666:HOH:O	2.20	0.42
1:D:41:PHE:HA	1:D:44:ARG:HH12	1.84	0.42
1:D:289:ALA:HB1	1:D:386:VAL:CG1	2.49	0.42
1:A:88:PHE:HB3	1:A:90:GLU:OE1	2.19	0.42
1:B:303:TRP:CD1	1:B:326:LYS:HD2	2.54	0.42
1:C:46:THR:HG22	1:C:48:ASN:HD21	1.82	0.42
1:C:120:TRP:CD2	1:C:122:GLN:HB2	2.53	0.42
1:C:328:ILE:HB	2:C:622:HOH:O	2.18	0.42
1:E:274:VAL:HB	1:E:275:PRO:HD3	2.00	0.42
1:F:279:SER:O	1:F:319:LYS:HD2	2.19	0.42
1:A:154:HIS:HD2	1:A:156:SER:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PHE:HD2	1:A:377:GLY:HA3	1.84	0.42
1:E:307:PRO:HB2	1:E:334:MET:HG3	2.00	0.42
1:F:110:LYS:HE2	2:F:643:HOH:O	2.18	0.42
1:C:51:ASN:C	1:C:51:ASN:ND2	2.67	0.42
1:C:223:SER:OG	1:C:346:HIS:HB2	2.20	0.42
1:F:118:GLN:HE21	1:F:118:GLN:HB3	1.61	0.42
1:A:154:HIS:CG	1:A:155:PRO:HD2	2.55	0.42
1:E:270:LEU:C	1:E:270:LEU:CD2	2.92	0.42
1:F:319:LYS:O	1:F:319:LYS:HG3	2.17	0.42
1:A:98:GLN:HA	1:A:98:GLN:NE2	2.34	0.42
1:A:340:MET:HE1	1:A:347:PHE:CG	2.55	0.42
1:B:172:THR:HG22	1:B:383:GLU:CD	2.43	0.42
1:E:158:LYS:HD3	1:F:175:ARG:HD2	2.02	0.42
1:F:67:ILE:HA	1:F:335:SER:HA	2.02	0.42
1:C:303:TRP:CZ2	1:C:322:LEU:HD21	2.55	0.42
1:E:103:MET:HG3	2:E:534:HOH:O	2.20	0.42
1:B:390:VAL:CG1	1:B:391:PRO:HD2	2.50	0.42
1:D:274:VAL:HB	1:D:275:PRO:HD3	2.01	0.42
1:A:294:LYS:HE2	2:A:543:HOH:O	2.20	0.41
1:B:51:ASN:ND2	1:B:54:LEU:HD12	2.35	0.41
1:B:245:THR:CG2	2:B:483:HOH:O	2.67	0.41
1:E:197:THR:C	1:E:199:VAL:H	2.27	0.41
1:F:105:VAL:CB	1:F:106:PRO:HD3	2.45	0.41
1:A:73:TYR:CD1	1:A:104:GLU:HG2	2.55	0.41
1:A:328:ILE:N	1:A:329:PRO:CD	2.83	0.41
1:B:80:LYS:NZ	2:B:611:HOH:O	2.53	0.41
1:C:113:ALA:HB2	1:C:192:ILE:HD11	2.02	0.41
1:C:141:PRO:HB2	1:C:145:PHE:HB3	2.02	0.41
1:C:165:HIS:HE1	1:D:161:GLY:O	2.03	0.41
1:D:162:VAL:O	1:D:162:VAL:HG23	2.21	0.41
1:F:69:GLN:HG2	1:F:70:ARG:N	2.33	0.41
1:F:76:GLU:HG2	1:F:80:LYS:HG3	2.01	0.41
1:F:178:LYS:HD2	1:F:242:ILE:HG22	2.02	0.41
1:A:105:VAL:CB	1:A:106:PRO:HD3	2.45	0.41
1:A:201:PHE:CD1	1:A:201:PHE:C	2.97	0.41
1:F:210:ASP:OD2	1:F:211:SER:N	2.51	0.41
1:A:325:THR:HA	1:A:328:ILE:HG12	2.01	0.41
1:B:60:ARG:HH21	1:B:61:ILE:CG1	2.27	0.41
1:B:132:PHE:CE1	1:B:143:ALA:HB3	2.56	0.41
1:B:137:THR:HB	1:B:163:PHE:CD1	2.55	0.41
1:C:46:THR:HG21	1:C:204:PRO:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:SER:C	1:C:195:GLU:HG2	2.45	0.41
1:F:88:PHE:H	1:F:90:GLU:CD	2.29	0.41
1:A:357:LEU:HD11	2:A:666:HOH:O	2.20	0.41
1:B:340:MET:N	1:B:344:CYS:SG	2.90	0.41
1:C:373:LEU:HB3	1:C:385:VAL:HB	2.03	0.41
1:E:185:ARG:HD2	2:E:551:HOH:O	2.20	0.41
1:E:251:PRO:O	1:E:252:ASN:C	2.63	0.41
1:A:256:ALA:HB3	1:A:380:LEU:HD12	2.02	0.41
1:F:201:PHE:HA	1:F:215:GLN:HE22	1.86	0.41
1:F:345:VAL:HG11	1:F:373:LEU:HD21	2.02	0.41
1:A:283:GLU:CD	1:A:298:TRP:HE1	2.28	0.41
1:B:377:GLY:O	1:B:378:PRO:C	2.64	0.41
1:C:172:THR:CB	1:C:383:GLU:OE2	2.68	0.41
1:D:31:ASN:HB3	2:D:628:HOH:O	2.19	0.41
1:D:373:LEU:C	1:D:373:LEU:HD23	2.46	0.41
1:F:28:ASN:O	1:F:29:PRO:C	2.63	0.41
1:B:19:ALA:HB2	1:B:182:GLU:HG3	2.02	0.41
1:D:132:PHE:CD2	1:D:147:VAL:HG21	2.55	0.41
1:B:330:THR:HA	1:B:348:ILE:CD1	2.50	0.41
1:C:133:CYS:CB	1:C:162:VAL:HG13	2.51	0.41
1:C:344:CYS:HB2	2:C:440:HOH:O	2.20	0.41
1:D:74:LEU:HD11	1:D:198:ALA:HA	2.03	0.41
1:D:105:VAL:HG13	1:D:194:SER:HB3	2.03	0.41
1:D:310:ARG:NH1	1:D:310:ARG:CG	2.81	0.41
1:E:361:CYS:HB3	1:E:367:GLY:N	2.36	0.41
1:E:381:THR:O	1:E:382:ILE:HD13	2.20	0.41
1:F:69:GLN:CG	1:F:70:ARG:N	2.83	0.41
1:D:302:PHE:CZ	1:D:371:GLY:HA3	2.56	0.41
1:E:90:GLU:H	1:E:90:GLU:CD	2.29	0.41
1:A:168:PHE:CD1	1:A:168:PHE:C	2.99	0.40
1:A:256:ALA:HB3	1:A:380:LEU:HD13	2.03	0.40
1:B:59:LYS:HE2	1:B:63:GLU:OE2	2.21	0.40
1:C:141:PRO:HB2	1:C:145:PHE:CB	2.51	0.40
1:C:325:THR:HA	1:C:328:ILE:CD1	2.51	0.40
1:E:156:SER:HA	1:F:247:GLN:O	2.21	0.40
1:A:340:MET:HE3	1:A:340:MET:HB2	1.93	0.40
1:E:58:PHE:HD2	1:E:212:LEU:CD1	2.34	0.40
1:E:196:THR:HA	1:E:220:ASP:CG	2.46	0.40
1:E:232:ILE:CG2	1:E:236:GLU:HG3	2.51	0.40
1:B:282:ILE:HG23	1:B:283:GLU:N	2.36	0.40
1:D:241:GLU:HB2	1:D:388:LYS:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:PHE:O	1:E:13:GLN:HB2	2.21	0.40
1:E:60:ARG:HH11	1:E:60:ARG:HG3	1.87	0.40
1:E:104:GLU:HA	1:E:104:GLU:OE1	2.21	0.40
1:E:260:LYS:O	1:E:266:LEU:HA	2.21	0.40
1:F:138:PRO:C	1:F:139:ASP:CG	2.89	0.40
1:A:18:PHE:CE1	1:A:243:VAL:HG22	2.57	0.40
1:A:290:PHE:CZ	1:A:301:LEU:HD23	2.57	0.40
1:C:81:LYS:HB3	1:C:81:LYS:HE2	1.82	0.40
1:D:293:PHE:O	1:D:295:ILE:HG13	2.20	0.40
1:E:56:ASP:CG	1:E:57:LYS:N	2.79	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	387/397 (98%)	359 (93%)	25 (6%)	3 (1%)	16	12
1	B	387/397 (98%)	359 (93%)	26 (7%)	2 (0%)	24	22
1	C	209/397 (53%)	199 (95%)	8 (4%)	2 (1%)	12	8
1	E	16/397 (4%)	13 (81%)	2 (12%)	1 (6%)	1	0
1	F	72/397 (18%)	66 (92%)	5 (7%)	1 (1%)	9	5
All	All	1071/1985 (54%)	996 (93%)	66 (6%)	9 (1%)	16	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	VAL
1	E	50	HIS
1	A	234	GLN
1	A	324	PRO

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Mol	Chain	Res	Type
1	B	89	VAL
1	C	17	GLY
1	F	379	GLY
1	B	378	PRO
1	C	89	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	321/325 (99%)	293 (91%)	28 (9%)	9	6
1	B	321/325 (99%)	298 (93%)	23 (7%)	13	10
1	C	321/325 (99%)	284 (88%)	37 (12%)	5	3
1	D	321/325 (99%)	295 (92%)	26 (8%)	11	8
1	E	321/325 (99%)	297 (92%)	24 (8%)	12	9
1	F	321/325 (99%)	292 (91%)	29 (9%)	9	6
All	All	1926/1950 (99%)	1759 (91%)	167 (9%)	9	6

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	18	PHE
1	A	26	THR
1	A	45	ILE
1	A	49	GLU
1	A	57	LYS
1	A	69	GLN
1	A	89	VAL
1	A	90	GLU
1	A	94	LEU
1	A	101	LEU
1	A	131	ILE
1	A	146	GLU

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Mol	Chain	Res	Type
1	A	153	LEU
1	A	159	ARG
1	A	162	VAL
1	A	172	THR
1	A	230	ASP
1	A	266	LEU
1	A	287	VAL
1	A	301	LEU
1	A	320	LEU
1	A	368	LEU
1	A	369	GLU
1	A	378	PRO
1	A	380	LEU
1	A	381	THR
1	A	388	LYS
1	B	10	ARG
1	B	20	SER
1	B	26	THR
1	B	80	LYS
1	B	81	LYS
1	B	91	VAL
1	B	94	LEU
1	B	98	GLN
1	B	101	LEU
1	B	103	MET
1	B	130	LEU
1	B	172	THR
1	B	173	VAL
1	B	254	GLU
1	B	269	GLN
1	B	270	LEU
1	B	284	ASN
1	B	301	LEU
1	B	357	LEU
1	B	380	LEU
1	B	388	LYS
1	B	392	ILE
1	B	393	GLN
1	C	7	GLU
1	C	10	ARG
1	C	26	THR
1	C	33	VAL

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Mol	Chain	Res	Type
1	C	45	ILE
1	C	52	THR
1	C	56	ASP
1	C	69	GLN
1	C	84	ASP
1	C	89	VAL
1	C	94	LEU
1	C	101	LEU
1	C	130	LEU
1	C	149	LYS
1	C	150	LEU
1	C	153	LEU
1	C	162	VAL
1	C	172	THR
1	C	173	VAL
1	C	196	THR
1	C	200	THR
1	C	212	LEU
1	C	250	VAL
1	C	276	ASP
1	C	287	VAL
1	C	294	LYS
1	C	300	LYS
1	C	301	LEU
1	C	319	LYS
1	C	320	LEU
1	C	323	ASP
1	C	357	LEU
1	C	363	THR
1	C	368	LEU
1	C	369	GLU
1	C	381	THR
1	C	388	LYS
1	D	10	ARG
1	D	44	ARG
1	D	49	GLU
1	D	51	ASN
1	D	53	GLU
1	D	59	LYS
1	D	61	ILE
1	D	85	VAL
1	D	94	LEU

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Mol	Chain	Res	Type
1	D	98	GLN
1	D	118	GLN
1	D	137	THR
1	D	140	LEU
1	D	162	VAL
1	D	172	THR
1	D	206	GLU
1	D	210	ASP
1	D	266	LEU
1	D	269	GLN
1	D	270	LEU
1	D	301	LEU
1	D	315	ARG
1	D	357	LEU
1	D	368	LEU
1	D	392	ILE
1	D	393	GLN
1	E	7	GLU
1	E	10	ARG
1	E	26	THR
1	E	34	ASP
1	E	35	GLN
1	E	45	ILE
1	E	49	GLU
1	E	51	ASN
1	E	60	ARG
1	E	94	LEU
1	E	98	GLN
1	E	153	LEU
1	E	162	VAL
1	E	173	VAL
1	E	223	SER
1	E	232	ILE
1	E	250	VAL
1	E	252	ASN
1	E	266	LEU
1	E	276	ASP
1	E	284	ASN
1	E	301	LEU
1	E	320	LEU
1	E	345	VAL
1	F	7	GLU

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Mol	Chain	Res	Type
1	F	10	ARG
1	F	12	LEU
1	F	26	THR
1	F	49	GLU
1	F	52	THR
1	F	57	LYS
1	F	98	GLN
1	F	101	LEU
1	F	118	GLN
1	F	130	LEU
1	F	139	ASP
1	F	159	ARG
1	F	173	VAL
1	F	225	LEU
1	F	234	GLN
1	F	266	LEU
1	F	276	ASP
1	F	281	ASN
1	F	297	ASP
1	F	300	LYS
1	F	301	LEU
1	F	310	ARG
1	F	319	LYS
1	F	345	VAL
1	F	354	LYS
1	F	357	LEU
1	F	369	GLU
1	F	393	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	69	GLN
1	A	98	GLN
1	A	154	HIS
1	A	164	GLN
1	A	208	HIS
1	A	215	GLN
1	A	252	ASN
1	A	332	HIS
1	A	351	GLN

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Mol	Chain	Res	Type
1	B	28	ASN
1	B	48	ASN
1	B	51	ASN
1	B	98	GLN
1	B	129	HIS
1	B	154	HIS
1	B	183	ASN
1	B	215	GLN
1	B	234	GLN
1	B	346	HIS
1	B	351	GLN
1	B	393	GLN
1	C	35	GLN
1	C	48	ASN
1	C	51	ASN
1	C	69	GLN
1	C	98	GLN
1	C	154	HIS
1	C	164	GLN
1	C	208	HIS
1	C	215	GLN
1	C	351	GLN
1	C	393	GLN
1	D	28	ASN
1	D	51	ASN
1	D	69	GLN
1	D	98	GLN
1	D	118	GLN
1	D	129	HIS
1	D	154	HIS
1	D	183	ASN
1	D	215	GLN
1	D	234	GLN
1	D	269	GLN
1	D	351	GLN
1	D	359	ASN
1	E	35	GLN
1	E	51	ASN
1	E	69	GLN
1	E	98	GLN
1	E	122	GLN
1	E	164	GLN

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Mol	Chain	Res	Type
1	E	208	HIS
1	E	215	GLN
1	E	252	ASN
1	E	321	ASN
1	E	346	HIS
1	E	351	GLN
1	E	358	GLN
1	F	13	GLN
1	F	28	ASN
1	F	51	ASN
1	F	98	GLN
1	F	118	GLN
1	F	129	HIS
1	F	154	HIS
1	F	164	GLN
1	F	183	ASN
1	F	215	GLN
1	F	234	GLN
1	F	281	ASN
1	F	351	GLN
1	F	393	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	389/397 (97%)	-1.38	0 100 100	20, 32, 48, 70	0
1	B	389/397 (97%)	-1.39	0 100 100	18, 30, 47, 68	0
1	C	389/397 (97%)	-1.41	0 100 100	16, 29, 48, 66	0
1	D	389/397 (97%)	-1.38	0 100 100	17, 32, 50, 64	0
1	E	389/397 (97%)	-1.36	0 100 100	22, 36, 51, 66	0
1	F	389/397 (97%)	-1.35	0 100 100	20, 36, 53, 67	0
All	All	2334/2382 (97%)	-1.38	0 100 100	16, 32, 50, 70	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.