



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:29 PM GMT

PDB ID : 4LQL
Title : Crystal structure of L-arabinose isomerase from *Lactobacillus fermentum* CGMCC2921
Authors : Xu, Z.
Deposited on : 2013-07-19
Resolution : 3.23 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

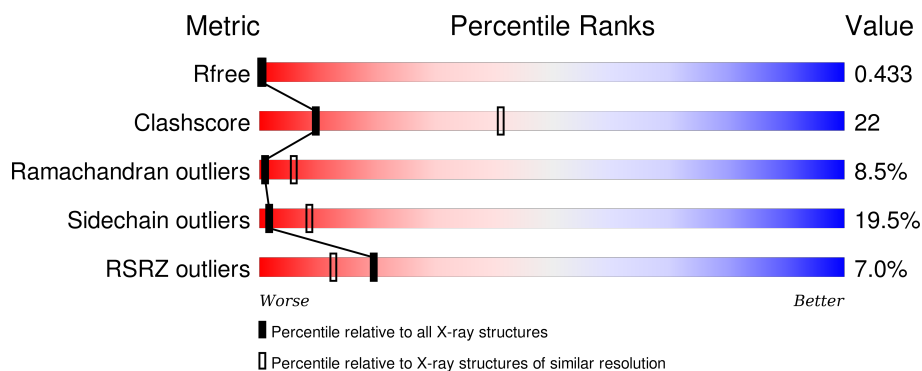
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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}	91344	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (3.28-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	474	<div> <div>8%</div> <div>57%</div> <div>36%</div> <div>7%</div> </div>
1	B	474	<div> <div>4%</div> <div>54%</div> <div>37%</div> <div>8%</div> </div>
1	C	474	<div> <div>5%</div> <div>61%</div> <div>33%</div> <div>5%</div> </div>
1	D	474	<div> <div>8%</div> <div>60%</div> <div>33%</div> <div>7%</div> </div>
1	E	474	<div> <div>8%</div> <div>51%</div> <div>40%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	474	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (8%), green (55%), yellow (39%), and orange (6%). The percentages are labeled below the corresponding segments.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18516 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.

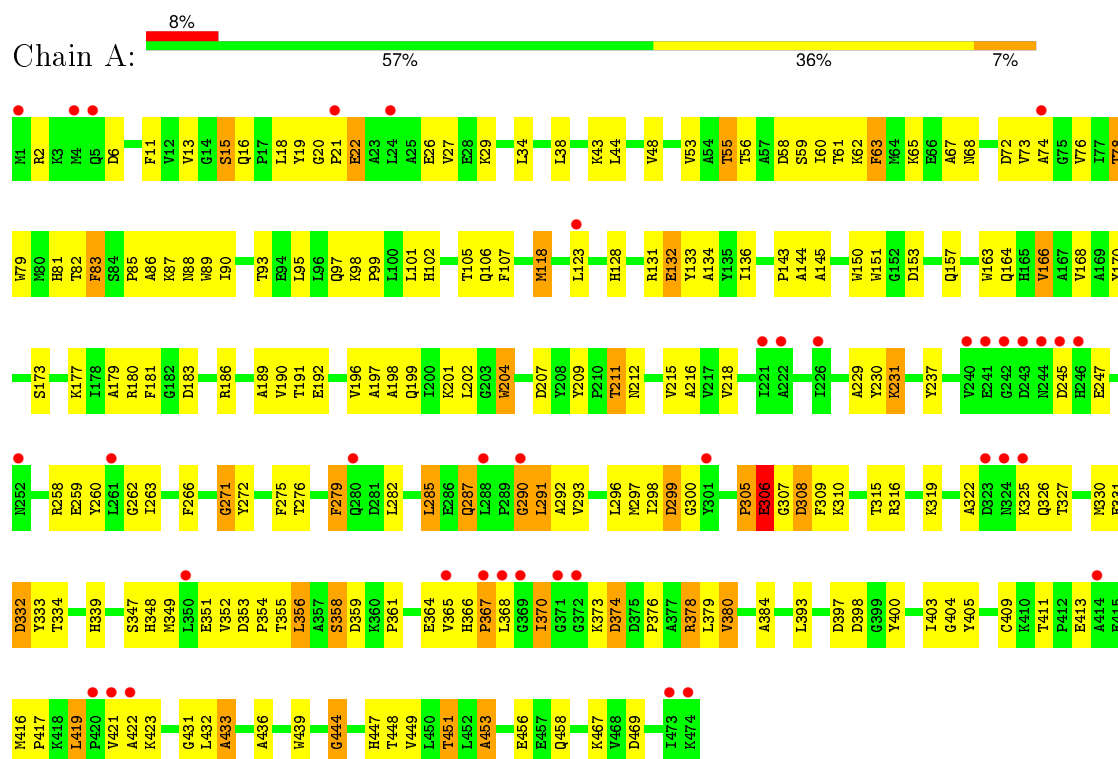
- Molecule 1 is a protein called L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3111	1999	538	566	8			
1	B	474	Total	C	N	O	S	0	0	0
			3130	2013	539	570	8			
1	C	474	Total	C	N	O	S	0	0	0
			3017	1936	517	556	8			
1	D	474	Total	C	N	O	S	0	0	0
			3111	1999	538	566	8			
1	E	474	Total	C	N	O	S	0	0	0
			3130	2013	539	570	8			
1	F	474	Total	C	N	O	S	0	0	0
			3017	1936	517	556	8			

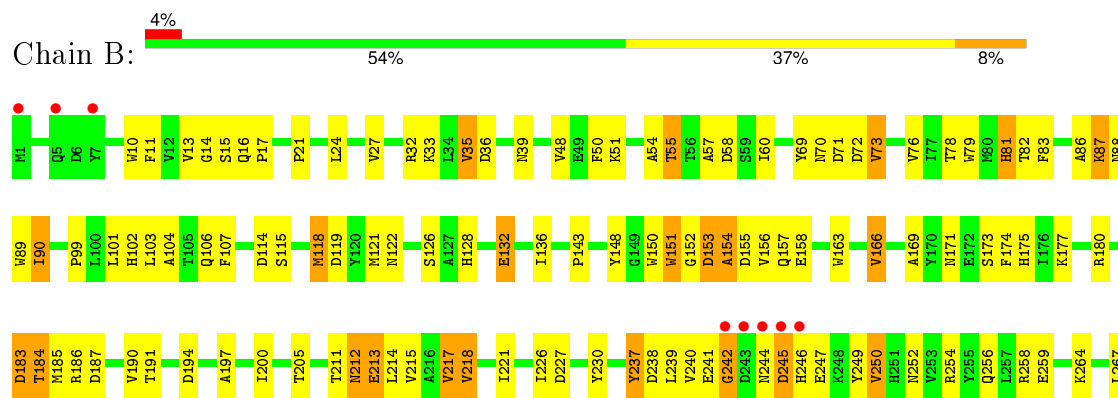
3 Residue-property plots

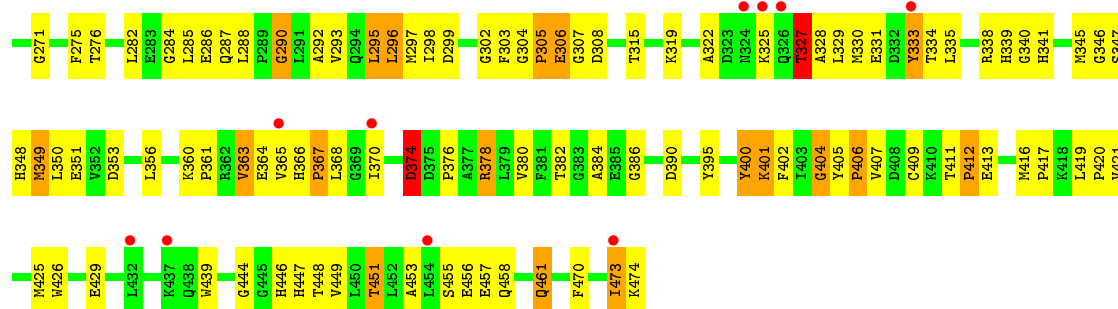
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: L-arabinose isomerase

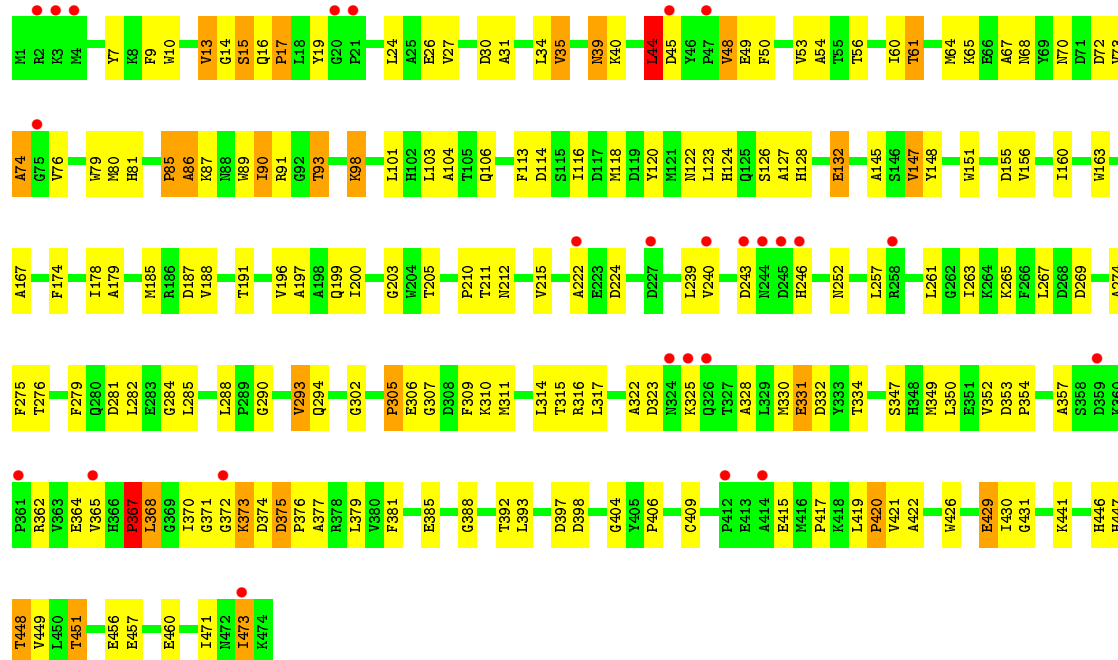


- Molecule 1: L-arabinose isomerase

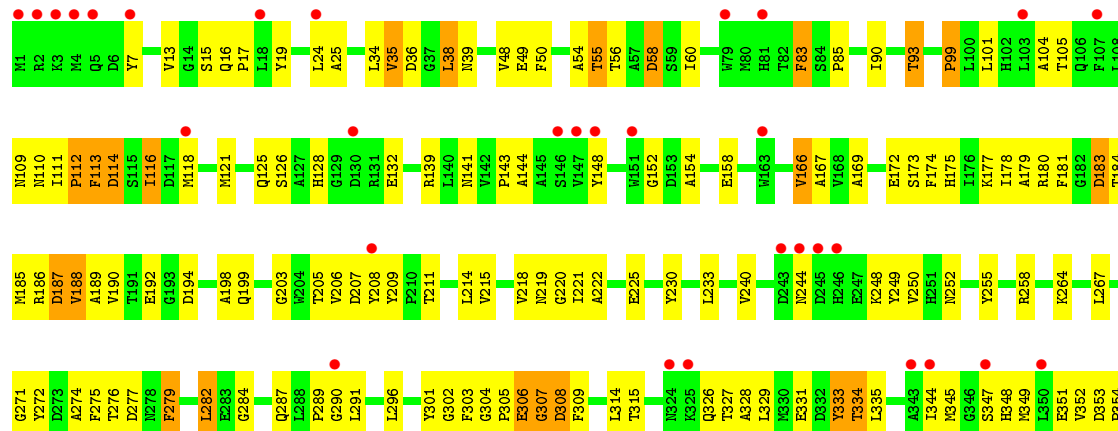


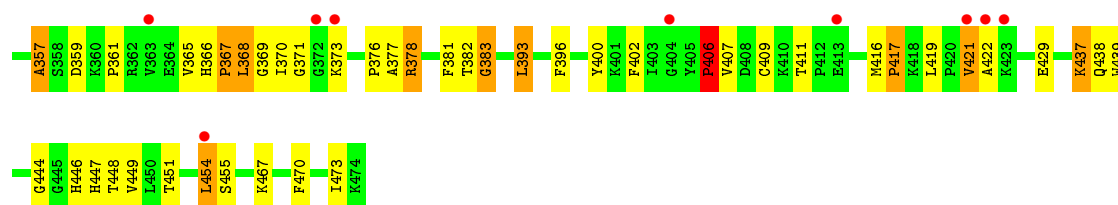


• Molecule 1: L-arabinose isomerase

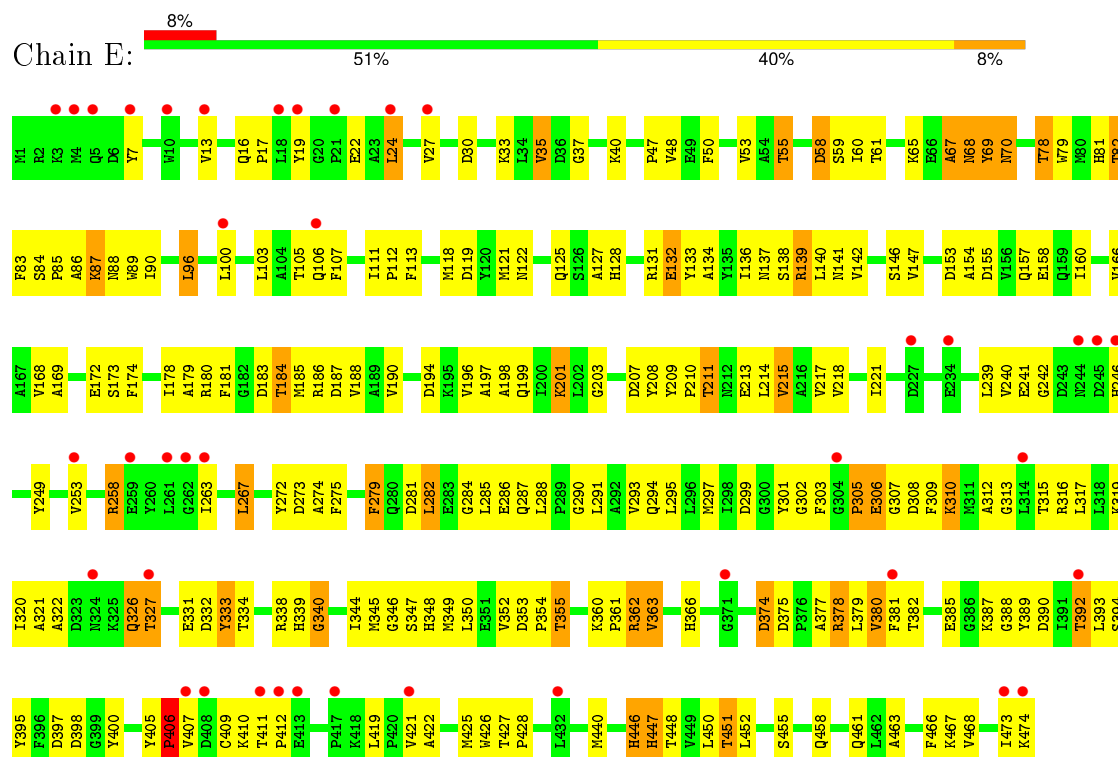


• Molecule 1: L-arabinose isomerase

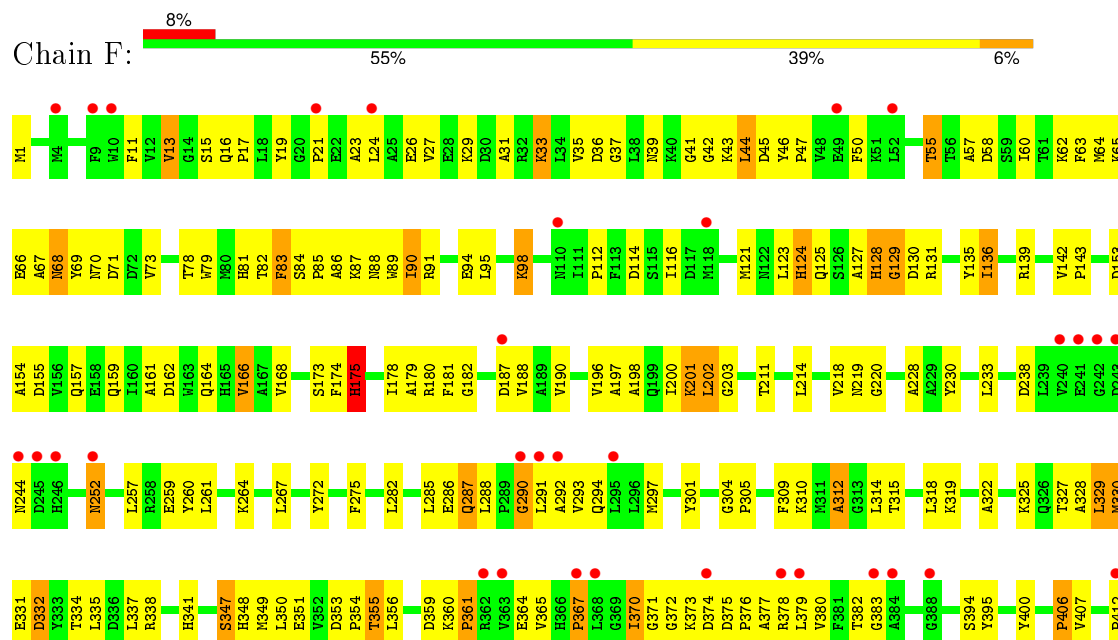




• Molecule 1: L-arabinose isomerase



• Molecule 1: L-arabinose isomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.20 Å 184.83 Å 186.35 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.85 – 3.23 44.85 – 3.23	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.85-3.23) 99.1 (44.85-3.23)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.25 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.314 , 0.432 0.315 , 0.433	Depositor DCC
R_{free} test set	2405 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	94.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 132.0	EDS
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 47542 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	18516	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.53	0/3156	0.80	1/4270 (0.0%)
1	B	0.58	0/3176	0.83	1/4293 (0.0%)
1	C	0.47	0/3060	0.72	0/4151
1	D	0.47	0/3156	0.72	0/4270
1	E	0.47	0/3176	0.70	1/4293 (0.0%)
1	F	0.50	0/3060	0.75	3/4151 (0.1%)
All	All	0.51	0/18784	0.76	6/25428 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	LEU	CA-CB-CG	6.87	131.09	115.30
1	F	95	LEU	CA-CB-CG	6.21	129.58	115.30
1	E	282	LEU	CA-CB-CG	5.97	129.04	115.30
1	B	404	GLY	N-CA-C	5.68	127.31	113.10
1	F	202	LEU	CA-CB-CG	5.24	127.35	115.30
1	F	175	HIS	CB-CA-C	-5.03	100.34	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	PRO	Peptide

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	3111	0	2557	132	0
1	B	3130	0	2581	141	0
1	C	3017	0	2377	123	0
1	D	3111	0	2557	116	0
1	E	3130	0	2581	155	0
1	F	3017	0	2377	148	0
All	All	18516	0	15030	752	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 22.

All (752) 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:C:294:GLN:HE21	1:C:352:VAL:H	1.20	0.89
1:A:439:TRP:NE1	1:A:444:GLY:O	2.07	0.88
1:A:308:ASP:OD2	1:A:447:HIS:ND1	2.07	0.87
1:A:85:PRO:HB3	1:C:188:VAL:HG22	1.58	0.86
1:A:192:GLU:O	1:A:310:LYS:NZ	2.09	0.85
1:C:305:PRO:O	1:C:307:GLY:N	2.11	0.82
1:F:331:GLU:OE2	1:F:348:HIS:NE2	2.12	0.82
1:F:35:VAL:O	1:F:39:ASN:ND2	2.14	0.80
1:C:322:ALA:HB1	1:C:325:LYS:HB2	1.65	0.79
1:F:73:VAL:O	1:F:98:LYS:NZ	2.17	0.77
1:E:338:ARG:O	1:E:340:GLY:N	2.18	0.77
1:B:194:ASP:HB3	1:B:197:ALA:HB3	1.66	0.77
1:B:416:MET:HB3	1:B:419:LEU:HB3	1.65	0.77
1:F:463:ALA:O	1:F:466:PHE:N	2.18	0.77
1:B:183:ASP:OD1	1:B:184:THR:N	2.16	0.77
1:A:285:LEU:O	1:A:373:LYS:NZ	2.15	0.76
1:D:331:GLU:HG3	1:D:447:HIS:HD2	1.51	0.76
1:D:308:ASP:OD2	1:D:447:HIS:ND1	2.17	0.76
1:A:331:GLU:OE2	1:A:348:HIS:NE2	2.19	0.76
1:A:183:ASP:OD2	1:E:180:ARG:NH2	2.19	0.76
1:E:282:LEU:HD11	1:E:288:LEU:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:GLU:OE2	1:E:348:HIS:NE2	2.20	0.75
1:B:406:PRO:HB2	1:B:474:LYS:HB2	1.69	0.74
1:C:67:ALA:HB1	1:C:73:VAL:HG11	1.70	0.74
1:A:199:GLN:NE2	1:F:87:LYS:O	2.20	0.74
1:C:106:GLN:NE2	1:C:124:HIS:O	2.20	0.73
1:E:361:PRO:O	1:E:363:VAL:N	2.20	0.73
1:E:409:CYS:HB2	1:E:426:TRP:HB3	1.70	0.73
1:F:458:GLN:HA	1:F:461:GLN:HE21	1.53	0.73
1:E:319:LYS:NZ	1:E:327:THR:O	2.21	0.73
1:D:166:VAL:O	1:D:169:ALA:N	2.22	0.73
1:F:463:ALA:O	1:F:467:LYS:N	2.19	0.72
1:E:86:ALA:O	1:E:89:TRP:N	2.20	0.72
1:E:446:HIS:HB3	1:F:128:HIS:HB3	1.71	0.72
1:F:364:GLU:HA	1:F:377:ALA:HA	1.71	0.72
1:B:455:SER:O	1:B:457:GLU:N	2.22	0.72
1:E:253:VAL:HG22	1:E:377:ALA:HB2	1.71	0.72
1:B:78:THR:O	1:B:103:LEU:N	2.19	0.72
1:A:451:THR:OG1	1:A:451:THR:O	2.08	0.71
1:C:64:MET:O	1:C:68:ASN:ND2	2.23	0.71
1:C:73:VAL:O	1:C:98:LYS:NZ	2.23	0.71
1:B:405:TYR:HA	1:B:473:ILE:O	1.91	0.71
1:E:137:ASN:O	1:E:139:ARG:N	2.25	0.70
1:D:357:ALA:HA	1:D:383:GLY:HA2	1.73	0.70
1:E:166:VAL:HG11	1:E:461:GLN:HB2	1.74	0.70
1:B:347:SER:OG	1:B:348:HIS:N	2.24	0.70
1:B:256:GLN:HA	1:B:259:GLU:HB2	1.73	0.70
1:A:15:SER:O	1:A:55:THR:HA	1.92	0.70
1:A:305:PRO:O	1:A:307:GLY:N	2.25	0.70
1:A:364:GLU:O	1:A:378:ARG:NH1	2.24	0.69
1:B:446:HIS:CD2	1:B:446:HIS:H	2.07	0.69
1:E:446:HIS:HE1	1:F:83:PHE:CZ	2.10	0.69
1:A:61:THR:O	1:A:65:LYS:HB2	1.94	0.68
1:B:221:ILE:O	1:B:258:ARG:NH2	2.26	0.68
1:A:358:SER:OG	1:A:359:ASP:N	2.26	0.68
1:A:131:ARG:NH1	1:C:332:ASP:OD1	2.26	0.68
1:B:104:ALA:HB3	1:B:148:TYR:HA	1.76	0.67
1:A:347:SER:OG	1:A:348:HIS:N	2.27	0.67
1:C:448:THR:OG1	1:C:449:VAL:N	2.27	0.66
1:B:87:LYS:HE3	1:E:199:GLN:OE1	1.96	0.66
1:A:319:LYS:NZ	1:A:327:THR:O	2.28	0.66
1:D:378:ARG:HG3	1:D:421:VAL:HG13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:LEU:HB2	1:D:373:LYS:HE3	1.78	0.66
1:A:332:ASP:O	1:B:128:HIS:HB3	1.95	0.66
1:B:16:GLN:HA	1:B:55:THR:HG22	1.77	0.66
1:A:73:VAL:O	1:A:98:LYS:HE2	1.94	0.66
1:D:54:ALA:HB1	1:D:60:ILE:HG12	1.76	0.66
1:F:125:GLN:OE1	1:F:128:HIS:NE2	2.28	0.65
1:B:345:MET:HA	1:B:425:MET:HA	1.79	0.65
1:B:227:ASP:HA	1:B:230:TYR:HB3	1.78	0.65
1:E:294:GLN:HE21	1:E:352:VAL:H	1.44	0.65
1:B:306:GLU:OE2	1:B:447:HIS:NE2	2.24	0.65
1:E:347:SER:OG	1:E:348:HIS:N	2.29	0.65
1:F:297:MET:HB3	1:F:353:ASP:CG	2.17	0.65
1:C:116:ILE:HG13	1:C:120:TYR:HB3	1.79	0.64
1:E:133:TYR:O	1:E:136:ILE:HG22	1.97	0.64
1:A:6:ASP:O	1:A:72:ASP:HB3	1.98	0.64
1:C:90:ILE:O	1:C:93:THR:N	2.31	0.64
1:E:313:GLY:O	1:E:317:LEU:N	2.28	0.64
1:A:118:MET:SD	1:A:118:MET:N	2.67	0.64
1:D:331:GLU:OE2	1:D:447:HIS:NE2	2.31	0.64
1:F:128:HIS:CD2	1:F:129:GLY:H	2.15	0.63
1:E:446:HIS:O	1:E:448:THR:N	2.30	0.63
1:A:199:GLN:HE22	1:F:87:LYS:HB3	1.63	0.63
1:A:376:PRO:O	1:A:378:ARG:NH2	2.30	0.63
1:F:309:PHE:HA	1:F:312:ALA:HB3	1.80	0.63
1:E:344:ILE:O	1:E:426:TRP:N	2.31	0.63
1:D:348:HIS:ND1	1:D:351:GLU:OE2	2.32	0.63
1:E:291:LEU:HB3	1:E:378:ARG:HA	1.81	0.63
1:E:79:TRP:NE1	1:E:105:THR:O	2.32	0.63
1:F:37:GLY:O	1:F:41:GLY:N	2.29	0.63
1:C:26:GLU:O	1:C:30:ASP:N	2.30	0.63
1:F:62:LYS:HA	1:F:65:LYS:HB2	1.81	0.62
1:B:27:VAL:HG12	1:B:81:HIS:CD2	2.34	0.62
1:F:297:MET:SD	1:F:353:ASP:HB2	2.38	0.62
1:B:366:HIS:O	1:B:368:LEU:N	2.32	0.62
1:D:35:VAL:HG21	1:D:50:PHE:HB2	1.80	0.62
1:F:35:VAL:HG21	1:F:50:PHE:HB2	1.81	0.62
1:F:121:MET:O	1:F:125:GLN:NE2	2.31	0.62
1:D:279:PHE:HD2	1:D:279:PHE:H	1.47	0.62
1:C:14:GLY:HA2	1:C:54:ALA:HB3	1.81	0.62
1:D:190:VAL:HG23	1:E:132:GLU:OE2	1.98	0.62
1:B:338:ARG:O	1:B:340:GLY:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:LEU:HD13	1:D:393:LEU:HD13	1.81	0.62
1:E:305:PRO:O	1:E:307:GLY:N	2.28	0.62
1:A:431:GLY:O	1:A:433:ALA:N	2.31	0.61
1:A:403:ILE:O	1:A:405:TYR:N	2.33	0.61
1:B:305:PRO:O	1:B:307:GLY:N	2.30	0.61
1:A:331:GLU:OE2	1:A:447:HIS:NE2	2.34	0.61
1:B:163:TRP:O	1:B:166:VAL:N	2.30	0.61
1:F:291:LEU:HA	1:F:294:GLN:OE1	2.01	0.61
1:C:457:GLU:HA	1:C:460:GLU:HB2	1.83	0.61
1:A:166:VAL:HG11	1:A:458:GLN:O	2.01	0.61
1:F:267:LEU:O	1:F:272:TYR:N	2.33	0.61
1:C:364:GLU:HA	1:C:377:ALA:HA	1.82	0.61
1:E:137:ASN:C	1:E:139:ARG:H	2.04	0.60
1:B:368:LEU:HD23	1:B:370:ILE:O	2.00	0.60
1:B:86:ALA:O	1:B:88:ASN:N	2.34	0.60
1:D:132:GLU:OE2	1:F:190:VAL:N	2.21	0.60
1:E:187:ASP:O	1:F:85:PRO:HB3	2.01	0.60
1:B:249:TYR:O	1:B:252:ASN:ND2	2.27	0.60
1:F:395:TYR:HB2	1:F:400:TYR:CE1	2.35	0.60
1:A:189:ALA:HB2	1:B:86:ALA:HB3	1.82	0.60
1:B:322:ALA:HB1	1:B:325:LYS:HB2	1.83	0.60
1:C:265:LYS:O	1:C:269:ASP:N	2.25	0.60
1:C:282:LEU:HD22	1:C:285:LEU:HD12	1.82	0.60
1:A:296:LEU:HA	1:A:299:ASP:HB2	1.84	0.60
1:B:86:ALA:O	1:B:89:TRP:N	2.27	0.60
1:E:127:ALA:O	1:E:131:ARG:NH1	2.34	0.60
1:B:14:GLY:O	1:B:15:SER:OG	2.20	0.59
1:B:333:TYR:H	1:B:346:GLY:HA2	1.66	0.59
1:D:36:ASP:HA	1:D:39:ASN:ND2	2.17	0.59
1:E:35:VAL:HG21	1:E:50:PHE:HB2	1.84	0.59
1:E:344:ILE:N	1:E:426:TRP:O	2.24	0.59
1:F:291:LEU:HB2	1:F:378:ARG:HA	1.85	0.59
1:A:128:HIS:ND1	1:C:332:ASP:O	2.35	0.59
1:E:140:LEU:O	1:E:142:VAL:N	2.35	0.59
1:B:186:ARG:HD3	1:D:208:TYR:O	2.03	0.59
1:C:179:ALA:H	1:C:275:PHE:HA	1.67	0.59
1:D:13:VAL:O	1:D:54:ALA:N	2.34	0.59
1:E:125:GLN:HB2	1:E:128:HIS:HE1	1.68	0.59
1:D:334:THR:O	1:D:345:MET:N	2.25	0.59
1:C:263:ILE:O	1:C:267:LEU:N	2.21	0.58
1:F:84:SER:HG	1:F:89:TRP:HE1	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ARG:HD2	1:D:206:VAL:CG1	2.32	0.58
1:B:153:ASP:O	1:B:156:VAL:N	2.36	0.58
1:D:306:GLU:C	1:D:308:ASP:H	2.07	0.58
1:D:184:THR:HA	1:D:307:GLY:HA3	1.86	0.58
1:C:27:VAL:HG13	1:C:123:LEU:HD11	1.84	0.58
1:F:322:ALA:HA	1:F:325:LYS:HB2	1.84	0.58
1:E:361:PRO:HD2	1:E:380:VAL:O	2.03	0.58
1:A:34:LEU:O	1:A:38:LEU:HG	2.02	0.58
1:D:58:ASP:OD2	1:D:58:ASP:N	2.35	0.58
1:E:390:ASP:O	1:E:405:TYR:N	2.36	0.58
1:A:333:TYR:HE1	1:A:348:HIS:HA	1.67	0.58
1:C:90:ILE:HG22	1:C:91:ARG:N	2.18	0.58
1:B:180:ARG:NH2	1:D:183:ASP:OD2	2.36	0.58
1:D:222:ALA:HB3	1:D:225:GLU:HB2	1.86	0.58
1:F:173:SER:C	1:F:175:HIS:H	2.05	0.58
1:A:101:LEU:HD22	1:A:163:TRP:CE3	2.39	0.58
1:B:245:ASP:O	1:B:246:HIS:ND1	2.36	0.58
1:A:347:SER:HB3	1:A:423:LYS:HB3	1.85	0.57
1:E:390:ASP:HB3	1:E:405:TYR:HB2	1.85	0.57
1:B:173:SER:C	1:B:175:HIS:H	2.07	0.57
1:E:111:ILE:O	1:E:113:PHE:N	2.38	0.57
1:F:406:PRO:HB2	1:F:474:LYS:HA	1.84	0.57
1:A:86:ALA:HA	1:A:89:TRP:HD1	1.69	0.57
1:C:199:GLN:CD	1:D:90:ILE:HG13	2.25	0.57
1:B:439:TRP:NE1	1:B:444:GLY:O	2.37	0.57
1:B:15:SER:OG	1:B:82:THR:OG1	2.22	0.57
1:C:311:MET:HA	1:C:314:LEU:HB3	1.87	0.57
1:A:164:GLN:O	1:A:168:VAL:HG23	2.03	0.57
1:D:296:LEU:O	1:D:301:TYR:HB2	2.04	0.57
1:D:173:SER:C	1:D:175:HIS:H	2.08	0.57
1:C:281:ASP:O	1:C:282:LEU:HD23	2.05	0.57
1:F:420:PRO:HG2	1:F:421:VAL:HG23	1.84	0.57
1:B:334:THR:OG1	1:B:335:LEU:N	2.38	0.57
1:D:16:GLN:HB3	1:D:19:TYR:CZ	2.40	0.57
1:F:125:GLN:HB2	1:F:128:HIS:HE2	1.69	0.57
1:A:150:TRP:HB3	1:A:153:ASP:HB2	1.87	0.57
1:D:407:VAL:HA	1:D:429:GLU:HB2	1.86	0.57
1:F:166:VAL:HG11	1:F:461:GLN:HB2	1.86	0.57
1:B:356:LEU:O	1:B:384:ALA:N	2.38	0.57
1:C:39:ASN:OD1	1:C:39:ASN:N	2.35	0.57
1:E:96:LEU:HD21	1:E:100:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:ARG:HG2	1:E:379:LEU:O	2.05	0.56
1:E:82:THR:OG1	1:E:83:PHE:N	2.34	0.56
1:C:330:MET:O	1:C:448:THR:HG23	2.05	0.56
1:E:360:LYS:HA	1:E:381:PHE:HB3	1.86	0.56
1:F:310:LYS:O	1:F:314:LEU:HB2	2.06	0.56
1:C:15:SER:OG	1:C:16:GLN:N	2.39	0.56
1:F:304:GLY:HA3	1:F:312:ALA:HB2	1.86	0.56
1:D:178:ILE:O	1:D:207:ASP:N	2.37	0.56
1:B:214:LEU:HD23	1:B:285:LEU:HD21	1.87	0.56
1:F:84:SER:OG	1:F:89:TRP:NE1	2.37	0.56
1:E:275:PHE:CE1	1:E:303:PHE:HB2	2.40	0.56
1:B:240:VAL:O	1:B:242:GLY:N	2.39	0.56
1:B:14:GLY:HA2	1:B:54:ALA:HB3	1.88	0.56
1:B:361:PRO:HD2	1:B:380:VAL:O	2.06	0.56
1:E:33:LYS:O	1:E:37:GLY:N	2.26	0.56
1:A:275:PHE:CE1	1:A:296:LEU:HD13	2.41	0.55
1:F:13:VAL:HA	1:F:79:TRP:O	2.05	0.55
1:C:328:ALA:HB1	1:C:353:ASP:HB3	1.86	0.55
1:B:194:ASP:N	1:B:400:TYR:OH	2.33	0.55
1:E:7:TYR:HD2	1:E:168:VAL:HG22	1.71	0.55
1:F:70:ASN:O	1:F:73:VAL:HG12	2.06	0.55
1:C:35:VAL:HG11	1:C:50:PHE:HB2	1.88	0.55
1:E:303:PHE:CZ	1:E:305:PRO:HA	2.41	0.55
1:D:180:ARG:N	1:D:207:ASP:O	2.36	0.55
1:C:239:LEU:HB3	1:C:243:ASP:HB2	1.88	0.55
1:D:104:ALA:HB3	1:D:148:TYR:CG	2.42	0.55
1:D:34:LEU:O	1:D:38:LEU:HB2	2.06	0.55
1:E:333:TYR:H	1:E:346:GLY:HA2	1.72	0.55
1:E:86:ALA:N	1:E:132:GLU:OE1	2.28	0.55
1:D:219:ASN:O	1:D:258:ARG:NH1	2.40	0.55
1:F:197:ALA:O	1:F:201:LYS:HB2	2.05	0.55
1:E:172:GLU:O	1:E:174:PHE:N	2.40	0.55
1:C:34:LEU:HA	1:C:151:TRP:CZ3	2.42	0.54
1:C:210:PRO:O	1:C:212:ASN:N	2.40	0.54
1:A:86:ALA:O	1:A:89:TRP:N	2.29	0.54
1:A:16:GLN:HG2	1:A:18:LEU:H	1.71	0.54
1:C:371:GLY:O	1:C:373:LYS:N	2.39	0.54
1:B:420:PRO:HD2	1:B:421:VAL:HG23	1.89	0.54
1:E:291:LEU:O	1:E:295:LEU:N	2.39	0.54
1:C:275:PHE:HZ	1:C:293:VAL:HG13	1.70	0.54
1:F:287:GLN:HG3	1:F:376:PRO:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:MET:O	1:C:122:ASN:N	2.41	0.54
1:E:294:GLN:HG2	1:E:354:PRO:HD3	1.89	0.54
1:D:179:ALA:HB2	1:D:272:TYR:CG	2.43	0.53
1:F:288:LEU:HD23	1:F:350:LEU:HD12	1.89	0.53
1:E:463:ALA:O	1:E:467:LYS:N	2.40	0.53
1:B:296:LEU:HA	1:B:299:ASP:HB2	1.90	0.53
1:B:10:TRP:CE2	1:B:51:LYS:HE3	2.42	0.53
1:B:10:TRP:CZ2	1:B:51:LYS:HE3	2.44	0.53
1:A:322:ALA:HB1	1:A:325:LYS:HB2	1.90	0.53
1:F:436:ALA:HA	1:F:439:TRP:HB3	1.90	0.53
1:A:128:HIS:HB3	1:C:332:ASP:HB3	1.90	0.53
1:E:392:THR:OG1	1:E:393:LEU:N	2.39	0.53
1:C:331:GLU:OE2	1:C:447:HIS:NE2	2.36	0.53
1:C:14:GLY:HA3	1:C:80:MET:HA	1.90	0.53
1:F:173:SER:O	1:F:175:HIS:N	2.42	0.53
1:B:70:ASN:O	1:B:72:ASP:N	2.42	0.53
1:B:402:PHE:O	1:B:470:PHE:HA	2.09	0.53
1:D:185:MET:HE3	1:D:188:VAL:HG21	1.91	0.53
1:B:276:THR:HG22	1:B:304:GLY:O	2.09	0.53
1:C:197:ALA:HB2	1:D:139:ARG:HH21	1.72	0.53
1:A:218:VAL:HG13	1:A:258:ARG:O	2.09	0.53
1:D:177:LYS:NZ	1:D:271:GLY:HA3	2.23	0.53
1:F:331:GLU:HG3	1:F:446:HIS:O	2.08	0.53
1:F:353:ASP:O	1:F:355:THR:N	2.41	0.53
1:A:322:ALA:HB1	1:A:325:LYS:CB	2.38	0.53
1:E:194:ASP:HB3	1:E:197:ALA:HB3	1.90	0.53
1:E:385:GLU:HA	1:E:410:LYS:HA	1.90	0.53
1:E:267:LEU:HD12	1:E:301:TYR:CD2	2.44	0.53
1:C:199:GLN:OE1	1:D:90:ILE:HG13	2.10	0.52
1:F:81:HIS:CE1	1:F:124:HIS:H	2.27	0.52
1:A:86:ALA:O	1:A:88:ASN:N	2.42	0.52
1:B:10:TRP:CD2	1:B:51:LYS:HG3	2.43	0.52
1:D:186:ARG:O	1:D:188:VAL:N	2.42	0.52
1:A:181:PHE:HE2	1:A:266:PHE:HE2	1.56	0.52
1:C:196:VAL:O	1:C:200:ILE:HG13	2.10	0.52
1:D:329:LEU:HA	1:D:449:VAL:HA	1.92	0.52
1:C:7:TYR:HB3	1:C:74:ALA:HB2	1.92	0.52
1:E:302:GLY:HA3	1:E:316:ARG:HB2	1.91	0.52
1:B:190:VAL:HG23	1:B:191:THR:HG23	1.92	0.52
1:B:303:PHE:CZ	1:B:305:PRO:HA	2.45	0.52
1:E:154:ALA:HA	1:E:157:GLN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:PRO:O	1:D:114:ASP:N	2.40	0.52
1:D:274:ALA:HA	1:D:302:GLY:O	2.09	0.52
1:D:368:LEU:HD22	1:D:376:PRO:HG3	1.91	0.52
1:A:436:ALA:O	1:A:439:TRP:N	2.40	0.52
1:E:446:HIS:CE1	1:F:83:PHE:CZ	2.96	0.52
1:A:275:PHE:CZ	1:A:293:VAL:HG22	2.45	0.52
1:A:291:LEU:HG	1:A:379:LEU:HB2	1.91	0.52
1:D:333:TYR:HD1	1:D:347:SER:O	1.92	0.52
1:E:172:GLU:C	1:E:174:PHE:H	2.11	0.51
1:A:105:THR:OG1	1:A:106:GLN:N	2.43	0.51
1:D:189:ALA:HB2	1:E:87:LYS:H	1.74	0.51
1:D:219:ASN:O	1:D:221:ILE:N	2.44	0.51
1:E:194:ASP:O	1:E:400:TYR:OH	2.28	0.51
1:D:85:PRO:HB3	1:F:187:ASP:O	2.09	0.51
1:A:180:ARG:HG2	1:A:276:THR:OG1	2.10	0.51
1:E:174:PHE:HA	1:E:203:GLY:HA3	1.91	0.51
1:C:156:VAL:O	1:C:160:ILE:HG13	2.10	0.51
1:B:87:LYS:HA	1:B:90:ILE:HG13	1.91	0.51
1:E:302:GLY:CA	1:E:316:ARG:HB2	2.40	0.51
1:B:328:ALA:O	1:B:449:VAL:HG13	2.10	0.51
1:F:252:ASN:ND2	1:F:287:GLN:OE1	2.43	0.51
1:A:133:TYR:O	1:A:136:ILE:HG22	2.11	0.51
1:D:128:HIS:HB3	1:F:332:ASP:O	2.11	0.51
1:E:293:VAL:HG12	1:E:297:MET:HG3	1.91	0.51
1:B:330:MET:O	1:B:448:THR:N	2.36	0.51
1:F:41:GLY:O	1:F:43:LYS:N	2.42	0.51
1:C:257:LEU:O	1:C:261:LEU:HD12	2.10	0.51
1:B:197:ALA:HA	1:B:200:ILE:HD12	1.93	0.51
1:E:198:ALA:HB2	1:E:400:TYR:OH	2.11	0.51
1:A:326:GLN:HB3	1:A:355:THR:O	2.11	0.51
1:D:177:LYS:HE3	1:D:271:GLY:O	2.11	0.51
1:F:315:THR:O	1:F:319:LYS:N	2.43	0.51
1:F:164:GLN:O	1:F:168:VAL:HG23	2.11	0.51
1:A:34:LEU:HA	1:A:151:TRP:CE3	2.45	0.51
1:A:26:GLU:HA	1:A:29:LYS:HB3	1.93	0.50
1:E:58:ASP:OD1	1:E:58:ASP:N	2.42	0.50
1:B:276:THR:HG21	1:B:307:GLY:O	2.11	0.50
1:F:15:SER:OG	1:F:16:GLN:N	2.44	0.50
1:A:16:GLN:HB3	1:A:19:TYR:CE1	2.46	0.50
1:F:395:TYR:HB2	1:F:400:TYR:HE1	1.76	0.50
1:D:172:GLU:O	1:D:175:HIS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:PHE:HA	1:D:209:TYR:O	2.10	0.50
1:B:33:LYS:HA	1:B:36:ASP:HB2	1.93	0.50
1:E:183:ASP:OD1	1:E:184:THR:N	2.29	0.50
1:C:178:ILE:HA	1:C:274:ALA:O	2.11	0.50
1:C:54:ALA:HB1	1:C:60:ILE:HD11	1.94	0.50
1:E:293:VAL:O	1:E:297:MET:N	2.45	0.50
1:A:285:LEU:HD22	1:A:287:GLN:O	2.12	0.50
1:E:319:LYS:O	1:E:322:ALA:N	2.33	0.50
1:A:128:HIS:HB2	1:C:446:HIS:HB2	1.93	0.50
1:E:201:LYS:NZ	1:E:467:LYS:O	2.40	0.50
1:B:10:TRP:CD2	1:B:73:VAL:HG11	2.46	0.50
1:B:446:HIS:HB3	1:C:128:HIS:HB2	1.93	0.50
1:A:259:GLU:O	1:A:263:ILE:N	2.44	0.50
1:C:16:GLN:HB3	1:C:19:TYR:CZ	2.47	0.50
1:E:60:ILE:HD13	1:E:89:TRP:CG	2.47	0.50
1:E:211:THR:O	1:E:215:VAL:HG23	2.12	0.50
1:E:24:LEU:O	1:E:27:VAL:HG22	2.11	0.50
1:A:131:ARG:O	1:A:134:ALA:HB3	2.11	0.49
1:D:417:PRO:HG2	1:E:113:PHE:O	2.12	0.49
1:A:153:ASP:O	1:A:157:GLN:HB2	2.12	0.49
1:C:197:ALA:HB2	1:D:139:ARG:NH2	2.27	0.49
1:F:294:GLN:HB3	1:F:354:PRO:HD3	1.94	0.49
1:C:331:GLU:HG3	1:C:447:HIS:CD2	2.48	0.49
1:D:331:GLU:HG3	1:D:447:HIS:CD2	2.40	0.49
1:B:378:ARG:HD3	1:B:420:PRO:O	2.12	0.49
1:D:214:LEU:O	1:D:218:VAL:HG23	2.12	0.49
1:F:159:GLN:HA	1:F:162:ASP:HB3	1.94	0.49
1:A:74:ALA:O	1:A:99:PRO:HD2	2.12	0.49
1:B:446:HIS:CB	1:C:128:HIS:HB2	2.41	0.49
1:A:79:TRP:NE1	1:A:105:THR:O	2.46	0.49
1:F:214:LEU:HG	1:F:214:LEU:O	2.13	0.49
1:C:385:GLU:HA	1:C:409:CYS:HB2	1.94	0.49
1:A:293:VAL:HG12	1:A:297:MET:HE2	1.95	0.49
1:A:20:GLY:O	1:A:22:GLU:N	2.45	0.49
1:C:352:VAL:HG21	1:C:422:ALA:O	2.13	0.49
1:F:26:GLU:HB2	1:F:123:LEU:HD11	1.94	0.49
1:D:111:ILE:O	1:D:113:PHE:N	2.45	0.49
1:F:429:GLU:O	1:F:431:GLY:N	2.44	0.49
1:F:33:LYS:O	1:F:37:GLY:N	2.46	0.49
1:C:31:ALA:O	1:C:34:LEU:N	2.45	0.49
1:F:128:HIS:HD2	1:F:129:GLY:H	1.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LYS:HB3	1:E:199:GLN:HE22	1.78	0.49
1:F:19:TYR:HB3	1:F:23:ALA:HB3	1.95	0.49
1:E:67:ALA:O	1:E:69:TYR:N	2.46	0.49
1:F:21:PRO:HA	1:F:24:LEU:HB2	1.94	0.49
1:A:287:GLN:NE2	1:A:376:PRO:HB3	2.27	0.49
1:C:362:ARG:HA	1:C:379:LEU:HD23	1.95	0.49
1:B:374:ASP:OD1	1:B:374:ASP:N	2.43	0.49
1:E:187:ASP:C	1:F:87:LYS:HG3	2.33	0.48
1:F:429:GLU:C	1:F:431:GLY:H	2.15	0.48
1:F:198:ALA:O	1:F:202:LEU:HB2	2.13	0.48
1:F:290:GLY:O	1:F:293:VAL:HG22	2.13	0.48
1:F:257:LEU:C	1:F:259:GLU:H	2.16	0.48
1:F:238:ASP:HB2	1:F:361:PRO:HB3	1.94	0.48
1:B:118:MET:O	1:B:122:ASN:ND2	2.46	0.48
1:B:87:LYS:O	1:E:199:GLN:NE2	2.46	0.48
1:D:186:ARG:C	1:D:188:VAL:H	2.17	0.48
1:C:404:GLY:N	1:C:471:ILE:O	2.46	0.48
1:A:279:PHE:CD1	1:A:370:ILE:HG23	2.48	0.48
1:A:271:GLY:O	1:A:272:TYR:CG	2.66	0.48
1:D:206:VAL:HG21	1:D:309:PHE:CG	2.48	0.48
1:E:169:ALA:HA	1:E:172:GLU:HB2	1.95	0.48
1:E:61:THR:O	1:E:65:LYS:HB2	2.14	0.48
1:E:179:ALA:HA	1:E:207:ASP:O	2.13	0.48
1:F:218:VAL:C	1:F:220:GLY:H	2.17	0.48
1:B:212:ASN:O	1:B:215:VAL:N	2.47	0.48
1:E:389:TYR:O	1:E:450:LEU:HA	2.14	0.48
1:F:201:LYS:NZ	1:F:467:LYS:O	2.47	0.48
1:C:65:LYS:HA	1:C:68:ASN:HD22	1.79	0.48
1:F:294:GLN:NE2	1:F:379:LEU:HB2	2.29	0.48
1:A:356:LEU:O	1:A:384:ALA:HB2	2.14	0.48
1:B:21:PRO:HA	1:B:24:LEU:HD12	1.96	0.48
1:D:306:GLU:O	1:D:308:ASP:N	2.47	0.48
1:F:455:SER:OG	1:F:458:GLN:HB2	2.14	0.48
1:C:9:PHE:C	1:C:10:TRP:HD1	2.17	0.48
1:E:214:LEU:O	1:E:217:VAL:N	2.47	0.48
1:B:405:TYR:HB3	1:B:439:TRP:CE3	2.49	0.47
1:E:405:TYR:HA	1:E:473:ILE:O	2.13	0.47
1:B:101:LEU:HD23	1:B:102:HIS:N	2.30	0.47
1:A:180:ARG:HD2	1:A:309:PHE:HB2	1.96	0.47
1:D:291:LEU:HB2	1:D:377:ALA:O	2.14	0.47
1:B:451:THR:C	1:B:453:ALA:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:TYR:O	1:B:401:LYS:HB2	2.14	0.47
1:F:128:HIS:O	1:F:131:ARG:N	2.47	0.47
1:E:190:VAL:HG12	1:F:135:TYR:HB2	1.96	0.47
1:B:221:ILE:HG21	1:B:258:ARG:HB2	1.96	0.47
1:B:169:ALA:C	1:B:171:ASN:H	2.16	0.47
1:B:177:LYS:HD3	1:B:271:GLY:O	2.14	0.47
1:B:390:ASP:O	1:B:404:GLY:HA2	2.14	0.47
1:F:309:PHE:HA	1:F:312:ALA:CB	2.44	0.47
1:F:267:LEU:HD21	1:F:275:PHE:HB3	1.97	0.47
1:D:359:ASP:HB2	1:D:361:PRO:HD3	1.95	0.47
1:A:352:VAL:HG21	1:A:422:ALA:O	2.15	0.47
1:C:79:TRP:CD1	1:C:80:MET:N	2.83	0.47
1:D:348:HIS:H	1:D:352:VAL:HG22	1.78	0.47
1:B:329:LEU:HA	1:B:449:VAL:HA	1.95	0.47
1:B:106:GLN:O	1:B:151:TRP:HD1	1.98	0.47
1:D:437:LYS:C	1:D:439:TRP:H	2.18	0.47
1:A:179:ALA:HA	1:A:207:ASP:O	2.15	0.47
1:D:83:PHE:HE1	1:D:132:GLU:HG3	1.79	0.47
1:B:406:PRO:CB	1:B:474:LYS:HB2	2.43	0.47
1:B:331:GLU:OE2	1:B:447:HIS:CD2	2.68	0.47
1:F:328:ALA:HB1	1:F:353:ASP:HB3	1.95	0.47
1:B:69:TYR:CD2	1:E:69:TYR:HB2	2.50	0.47
1:F:332:ASP:N	1:F:332:ASP:OD1	2.42	0.47
1:D:189:ALA:HB3	1:E:86:ALA:HB3	1.97	0.47
1:D:446:HIS:HB3	1:E:128:HIS:HB2	1.97	0.47
1:F:318:LEU:O	1:F:327:THR:HG21	2.14	0.47
1:B:295:LEU:O	1:B:298:ILE:N	2.40	0.47
1:F:91:ARG:HA	1:F:94:GLU:HB2	1.96	0.47
1:C:65:LYS:HA	1:C:68:ASN:ND2	2.30	0.47
1:D:416:MET:HA	1:D:419:LEU:HD23	1.97	0.47
1:B:226:ILE:O	1:B:230:TYR:N	2.48	0.47
1:A:90:ILE:HG12	1:A:136:ILE:HD11	1.97	0.47
1:A:90:ILE:HG21	1:F:200:ILE:HG12	1.96	0.47
1:D:215:VAL:HG21	1:D:284:GLY:HA3	1.97	0.47
1:C:429:GLU:O	1:C:431:GLY:N	2.43	0.47
1:A:212:ASN:O	1:A:215:VAL:HB	2.15	0.47
1:C:388:GLY:HA3	1:C:451:THR:O	2.15	0.47
1:C:103:LEU:HA	1:C:147:VAL:HG23	1.97	0.47
1:B:429:GLU:HB3	1:B:474:LYS:CG	2.45	0.47
1:B:154:ALA:O	1:B:158:GLU:N	2.48	0.47
1:F:348:HIS:ND1	1:F:351:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:HIS:O	1:C:126:SER:OG	2.19	0.46
1:D:255:TYR:HB2	1:D:287:GLN:NE2	2.30	0.46
1:A:198:ALA:O	1:A:202:LEU:HB2	2.15	0.46
1:E:294:GLN:HA	1:E:297:MET:HB2	1.96	0.46
1:C:104:ALA:HB3	1:C:148:TYR:CG	2.50	0.46
1:F:173:SER:C	1:F:175:HIS:N	2.69	0.46
1:A:198:ALA:HB2	1:A:400:TYR:OH	2.15	0.46
1:C:101:LEU:HD12	1:C:145:ALA:O	2.15	0.46
1:A:86:ALA:C	1:A:88:ASN:H	2.19	0.46
1:A:297:MET:SD	1:A:353:ASP:HB2	2.55	0.46
1:D:179:ALA:HA	1:D:207:ASP:O	2.15	0.46
1:F:17:PRO:HA	1:F:24:LEU:HD21	1.96	0.46
1:E:16:GLN:HA	1:E:55:THR:HG22	1.96	0.46
1:E:221:ILE:HB	1:E:258:ARG:NH2	2.30	0.46
1:A:353:ASP:HA	1:A:354:PRO:HD3	1.79	0.46
1:D:230:TYR:HA	1:D:233:LEU:HB2	1.96	0.46
1:A:315:THR:O	1:A:319:LYS:HG3	2.15	0.46
1:A:260:TYR:HB2	1:A:292:ALA:HA	1.98	0.46
1:F:64:MET:O	1:F:68:ASN:ND2	2.48	0.46
1:B:136:ILE:HA	1:B:136:ILE:HD12	1.64	0.46
1:D:249:TYR:HB3	1:D:252:ASN:HB2	1.98	0.46
1:C:179:ALA:O	1:C:276:THR:N	2.47	0.46
1:A:60:ILE:O	1:A:63:PHE:HB2	2.15	0.46
1:E:134:ALA:O	1:E:137:ASN:N	2.46	0.46
1:B:338:ARG:O	1:B:341:HIS:N	2.48	0.46
1:A:275:PHE:HE1	1:A:296:LEU:HD13	1.81	0.46
1:F:86:ALA:HA	1:F:89:TRP:HD1	1.81	0.46
1:C:240:VAL:H	1:C:243:ASP:HB2	1.81	0.46
1:E:69:TYR:HB3	1:E:70:ASN:H	1.65	0.46
1:F:44:LEU:HA	1:F:161:ALA:CB	2.46	0.46
1:B:173:SER:O	1:B:175:HIS:N	2.44	0.46
1:E:7:TYR:CD2	1:E:168:VAL:HG22	2.51	0.46
1:E:374:ASP:OD1	1:E:374:ASP:N	2.48	0.46
1:E:198:ALA:HB2	1:E:400:TYR:CZ	2.50	0.46
1:A:368:LEU:HD23	1:A:370:ILE:HB	1.98	0.46
1:E:331:GLU:HG3	1:E:446:HIS:HB2	1.96	0.45
1:D:113:PHE:HA	1:D:116:ILE:CD1	2.45	0.45
1:A:177:LYS:HB2	1:A:272:TYR:HA	1.98	0.45
1:F:153:ASP:OD1	1:F:155:ASP:N	2.49	0.45
1:F:347:SER:HB3	1:F:422:ALA:O	2.16	0.45
1:F:328:ALA:CB	1:F:353:ASP:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ALA:HB2	1:F:88:ASN:CG	2.37	0.45
1:A:101:LEU:HD13	1:A:163:TRP:CG	2.51	0.45
1:E:395:TYR:O	1:F:139:ARG:NH1	2.49	0.45
1:F:55:THR:O	1:F:55:THR:OG1	2.34	0.45
1:D:277:ASP:HB2	1:D:303:PHE:HE1	1.80	0.45
1:E:455:SER:O	1:E:458:GLN:N	2.49	0.45
1:B:256:GLN:O	1:B:292:ALA:HB2	2.15	0.45
1:D:252:ASN:O	1:D:287:GLN:NE2	2.49	0.45
1:F:350:LEU:HD21	1:F:376:PRO:HG2	1.99	0.45
1:B:282:LEU:HD11	1:B:288:LEU:HD13	1.98	0.45
1:D:353:ASP:HA	1:D:354:PRO:HD3	1.83	0.45
1:F:421:VAL:HG12	1:F:422:ALA:N	2.32	0.45
1:D:287:GLN:HA	1:D:373:LYS:HB3	1.99	0.45
1:E:294:GLN:HB3	1:E:354:PRO:HG3	1.98	0.45
1:F:294:GLN:HE22	1:F:379:LEU:H	1.65	0.45
1:A:56:THR:OG1	1:A:59:SER:N	2.41	0.45
1:B:319:LYS:HA	1:B:327:THR:HG21	1.98	0.45
1:A:361:PRO:HB2	1:A:380:VAL:HG13	1.98	0.45
1:E:309:PHE:O	1:E:312:ALA:HB3	2.16	0.45
1:B:32:ARG:O	1:B:35:VAL:HB	2.17	0.45
1:A:347:SER:HB2	1:A:352:VAL:HG21	1.98	0.45
1:C:90:ILE:HG21	1:D:199:GLN:HG2	1.98	0.45
1:E:274:ALA:HA	1:E:302:GLY:O	2.17	0.45
1:D:214:LEU:O	1:D:214:LEU:HG	2.17	0.45
1:F:153:ASP:OD1	1:F:154:ALA:N	2.50	0.45
1:B:187:ASP:HA	1:C:87:LYS:HD2	1.98	0.45
1:A:416:MET:HB2	1:A:419:LEU:HD22	1.99	0.45
1:B:305:PRO:C	1:B:307:GLY:H	2.15	0.45
1:A:245:ASP:C	1:A:247:GLU:H	2.20	0.45
1:F:69:TYR:O	1:F:71:ASP:N	2.50	0.45
1:E:242:GLY:O	1:E:249:TYR:HB2	2.16	0.45
1:C:215:VAL:HG21	1:C:284:GLY:HA3	1.99	0.45
1:E:333:TYR:HB2	1:E:347:SER:H	1.82	0.44
1:A:327:THR:HG23	1:A:451:THR:CB	2.48	0.44
1:B:244:ASN:HB2	1:B:247:GLU:CB	2.47	0.44
1:C:13:VAL:HG13	1:C:53:VAL:HA	1.98	0.44
1:E:188:VAL:HG22	1:F:85:PRO:HG3	1.98	0.44
1:B:153:ASP:O	1:B:157:GLN:N	2.44	0.44
1:C:10:TRP:CD1	1:C:49:GLU:HB2	2.52	0.44
1:A:85:PRO:HB2	1:C:187:ASP:O	2.17	0.44
1:E:333:TYR:CE2	1:F:128:HIS:HE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:446:HIS:CD2	1:E:446:HIS:N	2.84	0.44
1:E:125:GLN:HB2	1:E:128:HIS:CE1	2.52	0.44
1:C:240:VAL:HG12	1:C:243:ASP:CG	2.38	0.44
1:B:119:ASP:HA	1:B:122:ASN:HD21	1.82	0.44
1:D:277:ASP:HB2	1:D:303:PHE:CE1	2.52	0.44
1:F:451:THR:C	1:F:453:ALA:H	2.20	0.44
1:F:260:TYR:HB2	1:F:292:ALA:HA	1.99	0.44
1:E:406:PRO:HB2	1:E:474:LYS:HA	1.98	0.44
1:F:125:GLN:HB2	1:F:128:HIS:NE2	2.32	0.44
1:A:199:GLN:NE2	1:F:90:ILE:HD12	2.32	0.44
1:E:178:ILE:HA	1:E:274:ALA:O	2.18	0.44
1:C:70:ASN:CG	1:C:72:ASP:H	2.21	0.44
1:C:309:PHE:CG	1:C:310:LYS:N	2.85	0.44
1:F:356:LEU:O	1:F:383:GLY:HA2	2.17	0.44
1:B:395:TYR:HA	1:B:400:TYR:HA	2.00	0.44
1:D:166:VAL:O	1:D:167:ALA:C	2.55	0.44
1:F:287:GLN:NE2	1:F:376:PRO:HA	2.32	0.44
1:A:290:GLY:HA2	1:A:351:GLU:HG3	2.00	0.44
1:D:190:VAL:C	1:D:192:GLU:H	2.21	0.44
1:B:331:GLU:OE2	1:B:447:HIS:NE2	2.51	0.44
1:D:90:ILE:O	1:D:93:THR:N	2.51	0.44
1:B:119:ASP:HA	1:B:122:ASN:ND2	2.33	0.44
1:D:110:ASN:HA	1:F:337:LEU:H	1.83	0.44
1:E:319:LYS:O	1:E:321:ALA:N	2.51	0.44
1:E:137:ASN:C	1:E:139:ARG:N	2.71	0.44
1:A:245:ASP:O	1:A:247:GLU:N	2.50	0.44
1:E:345:MET:HA	1:E:425:MET:HA	2.00	0.44
1:E:349:MET:O	1:E:350:LEU:HD23	2.18	0.44
1:A:378:ARG:HE	1:A:378:ARG:HB3	1.54	0.44
1:B:333:TYR:HD2	1:B:333:TYR:HA	1.76	0.44
1:B:451:THR:O	1:B:451:THR:OG1	2.30	0.44
1:B:458:GLN:HA	1:B:461:GLN:HE21	1.83	0.44
1:E:147:VAL:HG21	1:E:160:ILE:HD13	1.99	0.44
1:C:352:VAL:O	1:C:381:PHE:HZ	2.01	0.44
1:A:183:ASP:HB3	1:E:208:TYR:CG	2.52	0.44
1:C:79:TRP:CZ2	1:C:106:GLN:HA	2.53	0.44
1:B:287:GLN:CD	1:B:376:PRO:HA	2.39	0.44
1:D:83:PHE:HB2	1:D:128:HIS:CE1	2.53	0.43
1:F:128:HIS:O	1:F:130:ASP:N	2.51	0.43
1:C:34:LEU:HA	1:C:151:TRP:CE3	2.53	0.43
1:E:215:VAL:HG22	1:E:285:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ALA:HB1	1:A:209:TYR:CG	2.53	0.43
1:D:105:THR:O	1:D:126:SER:OG	2.19	0.43
1:F:349:MET:SD	1:F:370:ILE:HD12	2.57	0.43
1:C:354:PRO:HA	1:C:381:PHE:CZ	2.53	0.43
1:C:60:ILE:HG21	1:C:89:TRP:CE3	2.53	0.43
1:C:61:THR:O	1:C:65:LYS:HB3	2.17	0.43
1:B:90:ILE:HD12	1:E:199:GLN:CD	2.38	0.43
1:C:179:ALA:HB3	1:C:275:PHE:HB2	1.99	0.43
1:C:86:ALA:HB2	1:C:132:GLU:HG3	1.99	0.43
1:D:15:SER:O	1:D:55:THR:HA	2.18	0.43
1:B:237:TYR:HB3	1:B:360:LYS:O	2.18	0.43
1:B:264:LYS:HE2	1:B:264:LYS:HB3	1.69	0.43
1:C:35:VAL:HG21	1:C:50:PHE:HB2	2.01	0.43
1:B:60:ILE:HD13	1:B:89:TRP:CD2	2.53	0.43
1:F:436:ALA:O	1:F:440:MET:HB2	2.17	0.43
1:B:215:VAL:HG11	1:B:284:GLY:HA3	2.00	0.43
1:D:154:ALA:O	1:D:158:GLU:HB2	2.18	0.43
1:D:335:LEU:HB3	1:D:344:ILE:HA	2.00	0.43
1:D:267:LEU:HD21	1:D:275:PHE:HB3	2.01	0.43
1:E:451:THR:OG1	1:E:451:THR:O	2.37	0.43
1:B:240:VAL:HG11	1:B:363:VAL:HG13	2.00	0.43
1:B:169:ALA:C	1:B:171:ASN:N	2.70	0.43
1:C:375:ASP:HA	1:C:376:PRO:HD3	1.79	0.43
1:A:173:SER:O	1:A:204:TRP:N	2.51	0.43
1:B:386:GLY:O	1:B:409:CYS:N	2.50	0.43
1:E:83:PHE:CE1	1:E:132:GLU:HG3	2.54	0.43
1:F:370:ILE:O	1:F:372:GLY:N	2.51	0.43
1:D:83:PHE:HZ	1:F:188:VAL:HG11	1.84	0.43
1:E:306:GLU:CD	1:E:348:HIS:HE1	2.21	0.43
1:E:187:ASP:HB3	1:F:87:LYS:HB2	2.00	0.43
1:B:254:ARG:O	1:B:258:ARG:N	2.47	0.43
1:D:446:HIS:O	1:D:448:THR:HG22	2.19	0.43
1:E:463:ALA:O	1:E:466:PHE:N	2.51	0.43
1:A:201:LYS:HB3	1:A:202:LEU:H	1.60	0.43
1:C:163:TRP:O	1:C:167:ALA:N	2.48	0.43
1:F:264:LYS:HG3	1:F:301:TYR:HE1	1.82	0.43
1:B:293:VAL:HG11	1:B:351:GLU:HG2	2.00	0.43
1:C:294:GLN:NE2	1:C:350:LEU:O	2.52	0.43
1:B:186:ARG:HB2	1:B:186:ARG:HE	1.36	0.43
1:D:406:PRO:O	1:D:429:GLU:HB3	2.19	0.43
1:E:272:TYR:O	1:E:274:ALA:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:GLU:O	1:C:417:PRO:HD3	2.18	0.43
1:A:199:GLN:HE21	1:F:90:ILE:HD12	1.83	0.43
1:F:27:VAL:HG12	1:F:81:HIS:ND1	2.34	0.43
1:F:44:LEU:HA	1:F:161:ALA:HB1	2.00	0.43
1:B:407:VAL:HG11	1:B:426:TRP:CD1	2.54	0.43
1:D:24:LEU:HA	1:D:24:LEU:HD23	1.89	0.43
1:F:434:GLU:O	1:F:437:LYS:HB2	2.19	0.43
1:A:128:HIS:HB2	1:C:446:HIS:CB	2.48	0.43
1:F:294:GLN:HB3	1:F:354:PRO:CD	2.49	0.43
1:A:237:TYR:CE2	1:A:379:LEU:HD11	2.54	0.43
1:E:67:ALA:O	1:E:68:ASN:C	2.57	0.43
1:C:222:ALA:C	1:C:224:ASP:H	2.21	0.43
1:A:186:ARG:HH11	1:E:209:TYR:HA	1.84	0.43
1:F:26:GLU:O	1:F:29:LYS:HB2	2.18	0.43
1:E:90:ILE:HD11	1:E:136:ILE:HD11	2.01	0.43
1:E:19:TYR:OH	1:E:125:GLN:OE1	2.33	0.43
1:C:288:LEU:HD21	1:C:349:MET:HE2	2.00	0.43
1:B:290:GLY:HA3	1:B:350:LEU:HD13	2.01	0.43
1:A:393:LEU:HD12	1:A:393:LEU:HA	1.62	0.43
1:E:333:TYR:N	1:E:346:GLY:HA2	2.33	0.42
1:F:364:GLU:HA	1:F:377:ALA:CA	2.45	0.42
1:A:325:LYS:HB3	1:A:453:ALA:HB1	2.01	0.42
1:C:274:ALA:HA	1:C:302:GLY:O	2.18	0.42
1:A:448:THR:HB	1:A:449:VAL:H	1.65	0.42
1:E:279:PHE:C	1:E:281:ASP:H	2.20	0.42
1:C:353:ASP:HA	1:C:354:PRO:HD2	1.77	0.42
1:A:189:ALA:CB	1:B:86:ALA:HB3	2.47	0.42
1:D:264:LYS:HB2	1:D:296:LEU:HD21	2.01	0.42
1:C:331:GLU:HG3	1:C:447:HIS:HD2	1.84	0.42
1:E:27:VAL:HA	1:E:30:ASP:HB2	2.02	0.42
1:D:109:ASN:C	1:F:337:LEU:HB2	2.39	0.42
1:E:84:SER:HA	1:E:85:PRO:HD3	1.73	0.42
1:C:352:VAL:HG11	1:C:422:ALA:HB3	2.01	0.42
1:E:136:ILE:HD12	1:E:136:ILE:HA	1.69	0.42
1:E:263:ILE:O	1:E:267:LEU:N	2.37	0.42
1:B:190:VAL:HG22	1:C:132:GLU:OE2	2.18	0.42
1:E:218:VAL:O	1:E:258:ARG:NE	2.28	0.42
1:D:369:GLY:O	1:D:371:GLY:N	2.51	0.42
1:F:329:LEU:O	1:F:330:MET:HB2	2.19	0.42
1:B:213:GLU:O	1:B:217:VAL:HG23	2.18	0.42
1:F:31:ALA:HB1	1:F:50:PHE:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:ALA:HB2	1:D:400:TYR:OH	2.20	0.42
1:E:310:LYS:HE3	1:E:310:LYS:HB2	1.60	0.42
1:A:439:TRP:CD1	1:A:439:TRP:O	2.73	0.42
1:B:446:HIS:CD2	1:B:446:HIS:N	2.82	0.42
1:F:33:LYS:HA	1:F:36:ASP:HB2	2.00	0.42
1:F:282:LEU:HD21	1:F:288:LEU:HD12	2.01	0.42
1:E:387:LYS:HB3	1:E:388:GLY:H	1.70	0.42
1:A:331:GLU:OE2	1:A:447:HIS:CD2	2.73	0.42
1:D:128:HIS:HB2	1:F:446:HIS:HB2	2.02	0.42
1:E:327:THR:HA	1:E:451:THR:HA	2.01	0.42
1:C:35:VAL:HG21	1:C:50:PHE:CG	2.54	0.42
1:F:180:ARG:O	1:F:182:GLY:N	2.53	0.42
1:A:229:ALA:C	1:A:231:LYS:H	2.23	0.42
1:C:357:ALA:HB2	1:C:381:PHE:CD1	2.55	0.42
1:F:11:PHE:CD1	1:F:35:VAL:HG22	2.54	0.42
1:F:291:LEU:HD12	1:F:379:LEU:HG	2.02	0.42
1:F:257:LEU:O	1:F:261:LEU:HD12	2.20	0.42
1:C:368:LEU:HD22	1:C:370:ILE:HG13	2.01	0.42
1:E:421:VAL:HG12	1:E:422:ALA:H	1.85	0.42
1:D:419:LEU:HG	1:D:421:VAL:O	2.20	0.42
1:C:31:ALA:O	1:C:35:VAL:N	2.48	0.42
1:F:86:ALA:C	1:F:88:ASN:H	2.22	0.42
1:A:330:MET:O	1:A:448:THR:OG1	2.36	0.42
1:B:217:VAL:HB	1:B:218:VAL:H	1.66	0.42
1:A:78:THR:O	1:A:102:HIS:HA	2.19	0.42
1:B:180:ARG:CZ	1:B:183:ASP:HA	2.50	0.42
1:E:381:PHE:HB2	1:E:382:THR:H	1.69	0.42
1:F:86:ALA:C	1:F:88:ASN:N	2.71	0.42
1:F:60:ILE:HD12	1:F:88:ASN:O	2.19	0.42
1:D:112:PRO:O	1:D:116:ILE:HG12	2.20	0.42
1:D:187:ASP:CB	1:E:85:PRO:HB2	2.50	0.42
1:E:419:LEU:C	1:E:421:VAL:H	2.24	0.42
1:D:402:PHE:O	1:D:470:PHE:HA	2.20	0.42
1:C:174:PHE:HA	1:C:203:GLY:HA3	2.02	0.42
1:B:413:GLU:HB2	1:C:113:PHE:CG	2.54	0.42
1:E:106:GLN:HG2	1:E:107:PHE:H	1.84	0.41
1:A:82:THR:OG1	1:A:83:PHE:N	2.43	0.41
1:A:16:GLN:CA	1:A:55:THR:HG22	2.50	0.41
1:D:279:PHE:N	1:D:279:PHE:CD2	2.88	0.41
1:B:154:ALA:O	1:B:158:GLU:HB2	2.20	0.41
1:F:230:TYR:O	1:F:233:LEU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:PRO:O	1:E:213:GLU:HB2	2.20	0.41
1:C:279:PHE:CD1	1:C:279:PHE:C	2.93	0.41
1:F:334:THR:HG22	1:F:335:LEU:N	2.35	0.41
1:A:191:THR:HB	1:A:308:ASP:HA	2.02	0.41
1:A:86:ALA:N	1:A:132:GLU:OE1	2.47	0.41
1:F:293:VAL:HG21	1:F:351:GLU:HG2	2.01	0.41
1:B:197:ALA:HA	1:B:200:ILE:CD1	2.50	0.41
1:D:185:MET:HB2	1:D:306:GLU:HB3	2.02	0.41
1:F:179:ALA:H	1:F:272:TYR:HB3	1.85	0.41
1:A:325:LYS:HB3	1:A:453:ALA:CB	2.51	0.41
1:A:349:MET:SD	1:A:370:ILE:HG21	2.61	0.41
1:E:78:THR:O	1:E:103:LEU:N	2.43	0.41
1:D:451:THR:OG1	1:D:454:LEU:HD12	2.20	0.41
1:A:85:PRO:HA	1:A:132:GLU:OE1	2.21	0.41
1:C:15:SER:H	1:C:54:ALA:HB3	1.85	0.41
1:B:60:ILE:HG21	1:B:89:TRP:CE3	2.55	0.41
1:C:39:ASN:ND2	1:C:48:VAL:H	2.18	0.41
1:C:9:PHE:O	1:C:48:VAL:HA	2.21	0.41
1:A:279:PHE:CE2	1:A:306:GLU:HG2	2.55	0.41
1:D:396:PHE:HA	1:E:139:ARG:NE	2.36	0.41
1:C:24:LEU:HA	1:C:27:VAL:HG22	2.03	0.41
1:C:275:PHE:CZ	1:C:293:VAL:HG13	2.53	0.41
1:F:375:ASP:HA	1:F:376:PRO:HD3	1.85	0.41
1:B:150:TRP:O	1:B:152:GLY:N	2.53	0.41
1:A:68:ASN:ND2	1:A:97:GLN:HB2	2.34	0.41
1:E:353:ASP:C	1:E:355:THR:H	2.24	0.41
1:D:381:PHE:H	1:D:422:ALA:HB2	1.85	0.41
1:D:83:PHE:H	1:D:125:GLN:HG3	1.85	0.41
1:F:62:LYS:O	1:F:66:GLU:HB2	2.21	0.41
1:F:367:PRO:HA	1:F:375:ASP:HB3	2.02	0.41
1:B:287:GLN:OE1	1:B:376:PRO:HA	2.21	0.41
1:D:276:THR:HG22	1:D:304:GLY:O	2.21	0.41
1:C:419:LEU:HD12	1:C:420:PRO:HD2	2.02	0.41
1:E:239:LEU:HA	1:E:362:ARG:HB3	2.01	0.41
1:E:375:ASP:N	1:E:375:ASP:OD2	2.53	0.41
1:E:308:ASP:OD2	1:E:447:HIS:ND1	2.52	0.41
1:D:35:VAL:HG11	1:D:49:GLU:C	2.41	0.41
1:A:259:GLU:O	1:A:262:GLY:N	2.52	0.41
1:D:437:LYS:O	1:D:439:TRP:N	2.54	0.41
1:F:338:ARG:HB3	1:F:341:HIS:H	1.85	0.41
1:E:306:GLU:OE2	1:E:447:HIS:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:MET:C	1:F:123:LEU:H	2.23	0.41
1:E:86:ALA:O	1:E:88:ASN:N	2.54	0.41
1:C:27:VAL:HG12	1:C:81:HIS:ND1	2.36	0.41
1:A:128:HIS:HB3	1:C:332:ASP:O	2.21	0.41
1:A:11:PHE:HZ	1:A:79:TRP:HE3	1.68	0.41
1:B:187:ASP:O	1:C:85:PRO:HB3	2.19	0.41
1:A:298:ILE:C	1:A:300:GLY:H	2.24	0.41
1:E:155:ASP:O	1:E:158:GLU:HB3	2.20	0.41
1:B:297:MET:SD	1:B:353:ASP:HB2	2.61	0.41
1:F:136:ILE:HD12	1:F:136:ILE:HA	1.89	0.41
1:C:30:ASP:O	1:C:34:LEU:N	2.54	0.41
1:A:190:VAL:HG23	1:B:132:GLU:HG2	2.03	0.41
1:B:70:ASN:C	1:B:72:ASP:N	2.75	0.40
1:A:59:SER:O	1:A:63:PHE:CG	2.74	0.40
1:B:237:TYR:O	1:B:239:LEU:N	2.55	0.40
1:F:348:HIS:O	1:F:421:VAL:HG11	2.21	0.40
1:D:331:GLU:OE2	1:D:447:HIS:CD2	2.74	0.40
1:D:396:PHE:HA	1:E:139:ARG:HE	1.86	0.40
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.85	0.40
1:C:367:PRO:HA	1:C:375:ASP:HA	2.03	0.40
1:C:44:LEU:HB3	1:C:45:ASP:H	1.62	0.40
1:E:326:GLN:HB2	1:E:452:LEU:HB2	2.02	0.40
1:F:26:GLU:HB3	1:F:123:LEU:HD21	2.04	0.40
1:C:126:SER:O	1:C:128:HIS:N	2.54	0.40
1:A:101:LEU:HD12	1:A:145:ALA:HB3	2.03	0.40
1:C:10:TRP:N	1:C:10:TRP:CD1	2.90	0.40
1:B:275:PHE:N	1:B:302:GLY:O	2.51	0.40
1:D:54:ALA:CB	1:D:60:ILE:HG12	2.49	0.40
1:E:352:VAL:O	1:E:381:PHE:HZ	2.04	0.40
1:C:215:VAL:HG22	1:C:285:LEU:HD23	2.03	0.40
1:E:172:GLU:C	1:E:174:PHE:N	2.75	0.40
1:B:155:ASP:HA	1:B:158:GLU:HB3	2.03	0.40
1:B:39:ASN:HD21	1:B:48:VAL:CB	2.35	0.40
1:B:79:TRP:NE1	1:B:126:SER:OG	2.55	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	472/474 (100%)	336 (71%)	89 (19%)	47 (10%)	1	4
1	B	472/474 (100%)	345 (73%)	86 (18%)	41 (9%)	1	5
1	C	472/474 (100%)	360 (76%)	80 (17%)	32 (7%)	1	11
1	D	472/474 (100%)	348 (74%)	84 (18%)	40 (8%)	1	6
1	E	472/474 (100%)	325 (69%)	108 (23%)	39 (8%)	1	6
1	F	472/474 (100%)	323 (68%)	107 (23%)	42 (9%)	1	5
All	All	2832/2844 (100%)	2037 (72%)	554 (20%)	241 (8%)	1	6

All (241) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PHE
1	A	305	PRO
1	A	306	GLU
1	A	356	LEU
1	A	367	PRO
1	A	404	GLY
1	A	453	ALA
1	B	50	PHE
1	B	183	ASP
1	B	212	ASN
1	B	217	VAL
1	B	218	VAL
1	B	241	GLU
1	B	339	HIS
1	B	349	MET
1	B	367	PRO
1	B	412	PRO
1	B	456	GLU
1	C	40	LYS
1	C	85	PRO

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Mol	Chain	Res	Type
1	C	211	THR
1	C	305	PRO
1	C	306	GLU
1	C	317	LEU
1	C	331	GLU
1	C	347	SER
1	C	372	GLY
1	C	373	LYS
1	D	17	PRO
1	D	113	PHE
1	D	116	ILE
1	D	141	ASN
1	D	248	LYS
1	D	305	PRO
1	D	308	ASP
1	D	367	PRO
1	D	467	LYS
1	E	68	ASN
1	E	141	ASN
1	E	273	ASP
1	E	299	ASP
1	E	305	PRO
1	E	339	HIS
1	E	362	ARG
1	E	366	HIS
1	E	380	VAL
1	E	427	THR
1	E	428	PRO
1	E	447	HIS
1	F	42	GLY
1	F	45	ASP
1	F	47	PRO
1	F	157	GLN
1	F	286	GLU
1	F	305	PRO
1	F	365	VAL
1	F	430	ILE
1	A	53	VAL
1	A	87	LYS
1	A	107	PHE
1	A	123	LEU
1	A	144	ALA

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Mol	Chain	Res	Type
1	A	170	TYR
1	A	196	VAL
1	A	216	ALA
1	A	231	LYS
1	A	271	GLY
1	A	299	ASP
1	A	374	ASP
1	A	432	LEU
1	A	444	GLY
1	B	71	ASP
1	B	83	PHE
1	B	87	LYS
1	B	90	ILE
1	B	151	TRP
1	B	213	GLU
1	B	238	ASP
1	B	296	LEU
1	B	305	PRO
1	B	306	GLU
1	B	308	ASP
1	B	401	LYS
1	B	417	PRO
1	C	44	LEU
1	C	90	ILE
1	C	127	ALA
1	C	316	ARG
1	D	25	ALA
1	D	35	VAL
1	D	144	ALA
1	D	174	PHE
1	D	187	ASP
1	D	220	GLY
1	D	244	ASN
1	D	307	GLY
1	D	328	ALA
1	D	383	GLY
1	D	417	PRO
1	D	444	GLY
1	E	81	HIS
1	E	82	THR
1	E	87	LYS
1	E	138	SER

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Mol	Chain	Res	Type
1	E	173	SER
1	E	241	GLU
1	E	286	GLU
1	E	320	ILE
1	E	327	THR
1	F	44	LEU
1	F	68	ASN
1	F	129	GLY
1	F	178	ILE
1	F	196	VAL
1	F	203	GLY
1	F	244	ASN
1	F	360	LYS
1	F	371	GLY
1	F	464	ARG
1	A	83	PHE
1	A	197	ALA
1	A	230	TYR
1	A	316	ARG
1	A	370	ILE
1	A	397	ASP
1	A	433	ALA
1	A	456	GLU
1	B	242	GLY
1	B	286	GLU
1	B	364	GLU
1	B	374	ASP
1	C	74	ALA
1	C	86	ALA
1	C	155	ASP
1	C	323	ASP
1	C	398	ASP
1	C	430	ILE
1	D	114	ASP
1	D	366	HIS
1	D	437	LYS
1	D	438	GLN
1	E	40	LYS
1	E	70	ASN
1	E	112	PRO
1	E	290	GLY
1	E	306	GLU

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Mol	Chain	Res	Type
1	E	334	THR
1	E	397	ASP
1	E	406	PRO
1	E	440	MET
1	F	67	ALA
1	F	174	PHE
1	F	219	ASN
1	F	359	ASP
1	F	373	LYS
1	F	412	PRO
1	F	442	TYR
1	A	2	ARG
1	A	62	LYS
1	A	67	ALA
1	A	204	TRP
1	A	211	THR
1	A	279	PHE
1	A	290	GLY
1	A	308	ASP
1	A	365	VAL
1	A	417	PRO
1	A	467	LYS
1	A	469	ASP
1	B	154	ALA
1	B	174	PHE
1	B	267	LEU
1	B	400	TYR
1	C	17	PRO
1	C	365	VAL
1	C	456	GLU
1	D	83	PHE
1	D	152	GLY
1	D	203	GLY
1	D	357	ALA
1	D	365	VAL
1	E	67	ALA
1	E	186	ARG
1	F	112	PRO
1	F	124	HIS
1	F	127	ALA
1	F	312	ALA
1	F	330	MET

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Mol	Chain	Res	Type
1	F	361	PRO
1	F	441	LYS
1	A	21	PRO
1	A	43	LYS
1	A	339	HIS
1	A	413	GLU
1	B	57	ALA
1	B	245	ASP
1	B	295	LEU
1	B	327	THR
1	C	191	THR
1	C	397	ASP
1	C	429	GLU
1	C	441	LYS
1	D	112	PRO
1	D	290	GLY
1	D	306	GLU
1	D	406	PRO
1	E	47	PRO
1	E	69	TYR
1	F	33	LYS
1	F	46	TYR
1	F	181	PHE
1	A	22	GLU
1	A	366	HIS
1	B	250	VAL
1	C	420	PRO
1	D	194	ASP
1	E	215	VAL
1	E	284	GLY
1	F	63	PHE
1	F	143	PRO
1	F	228	ALA
1	F	329	LEU
1	C	35	VAL
1	C	473	ILE
1	D	143	PRO
1	D	370	ILE
1	F	90	ILE
1	F	290	GLY
1	B	99	PRO
1	B	290	GLY

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Mol	Chain	Res	Type
1	D	99	PRO
1	D	289	PRO
1	E	35	VAL
1	E	340	GLY
1	B	35	VAL
1	C	367	PRO
1	D	166	VAL
1	F	367	PRO
1	B	143	PRO
1	E	407	VAL
1	C	290	GLY

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	194/393 (49%)	161 (83%)	33 (17%)	2	12
1	B	199/393 (51%)	161 (81%)	38 (19%)	2	9
1	C	173/393 (44%)	140 (81%)	33 (19%)	2	9
1	D	194/393 (49%)	157 (81%)	37 (19%)	2	9
1	E	199/393 (51%)	150 (75%)	49 (25%)	1	2
1	F	173/393 (44%)	142 (82%)	31 (18%)	2	11
All	All	1132/2358 (48%)	911 (80%)	221 (20%)	2	8

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	15	SER
1	A	27	VAL
1	A	44	LEU
1	A	48	VAL
1	A	55	THR
1	A	58	ASP

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Mol	Chain	Res	Type
1	A	76	VAL
1	A	78	THR
1	A	81	HIS
1	A	93	THR
1	A	118	MET
1	A	132	GLU
1	A	166	VAL
1	A	211	THR
1	A	282	LEU
1	A	285	LEU
1	A	287	GLN
1	A	291	LEU
1	A	306	GLU
1	A	332	ASP
1	A	334	THR
1	A	358	SER
1	A	367	PRO
1	A	374	ASP
1	A	378	ARG
1	A	380	VAL
1	A	398	ASP
1	A	409	CYS
1	A	411	THR
1	A	419	LEU
1	A	421	VAL
1	A	451	THR
1	B	11	PHE
1	B	13	VAL
1	B	17	PRO
1	B	55	THR
1	B	58	ASP
1	B	73	VAL
1	B	76	VAL
1	B	81	HIS
1	B	107	PHE
1	B	114	ASP
1	B	115	SER
1	B	118	MET
1	B	121	MET
1	B	132	GLU
1	B	153	ASP
1	B	166	VAL

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Mol	Chain	Res	Type
1	B	184	THR
1	B	185	MET
1	B	205	THR
1	B	211	THR
1	B	237	TYR
1	B	250	VAL
1	B	315	THR
1	B	327	THR
1	B	333	TYR
1	B	349	MET
1	B	363	VAL
1	B	365	VAL
1	B	367	PRO
1	B	374	ASP
1	B	378	ARG
1	B	382	THR
1	B	406	PRO
1	B	411	THR
1	B	412	PRO
1	B	451	THR
1	B	461	GLN
1	B	473	ILE
1	C	13	VAL
1	C	15	SER
1	C	17	PRO
1	C	39	ASN
1	C	44	LEU
1	C	48	VAL
1	C	56	THR
1	C	61	THR
1	C	76	VAL
1	C	93	THR
1	C	98	LYS
1	C	114	ASP
1	C	132	GLU
1	C	147	VAL
1	C	185	MET
1	C	205	THR
1	C	246	HIS
1	C	252	ASN
1	C	293	VAL
1	C	315	THR

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Mol	Chain	Res	Type
1	C	334	THR
1	C	367	PRO
1	C	368	LEU
1	C	374	ASP
1	C	375	ASP
1	C	392	THR
1	C	393	LEU
1	C	406	PRO
1	C	421	VAL
1	C	426	TRP
1	C	448	THR
1	C	451	THR
1	C	473	ILE
1	D	7	TYR
1	D	38	LEU
1	D	48	VAL
1	D	55	THR
1	D	56	THR
1	D	58	ASP
1	D	93	THR
1	D	99	PRO
1	D	101	LEU
1	D	118	MET
1	D	121	MET
1	D	183	ASP
1	D	188	VAL
1	D	205	THR
1	D	211	THR
1	D	240	VAL
1	D	250	VAL
1	D	279	PHE
1	D	282	LEU
1	D	315	THR
1	D	326	GLN
1	D	327	THR
1	D	333	TYR
1	D	334	THR
1	D	349	MET
1	D	367	PRO
1	D	368	LEU
1	D	378	ARG
1	D	382	THR

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Mol	Chain	Res	Type
1	D	393	LEU
1	D	406	PRO
1	D	409	CYS
1	D	411	THR
1	D	421	VAL
1	D	454	LEU
1	D	455	SER
1	D	473	ILE
1	E	13	VAL
1	E	17	PRO
1	E	22	GLU
1	E	24	LEU
1	E	48	VAL
1	E	53	VAL
1	E	55	THR
1	E	58	ASP
1	E	59	SER
1	E	78	THR
1	E	96	LEU
1	E	118	MET
1	E	119	ASP
1	E	121	MET
1	E	122	ASN
1	E	132	GLU
1	E	139	ARG
1	E	146	SER
1	E	153	ASP
1	E	181	PHE
1	E	184	THR
1	E	185	MET
1	E	196	VAL
1	E	201	LYS
1	E	211	THR
1	E	240	VAL
1	E	246	HIS
1	E	258	ARG
1	E	267	LEU
1	E	279	PHE
1	E	287	GLN
1	E	310	LYS
1	E	315	THR
1	E	326	GLN

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Mol	Chain	Res	Type
1	E	332	ASP
1	E	333	TYR
1	E	355	THR
1	E	363	VAL
1	E	374	ASP
1	E	378	ARG
1	E	392	THR
1	E	394	SER
1	E	398	ASP
1	E	406	PRO
1	E	411	THR
1	E	412	PRO
1	E	446	HIS
1	E	451	THR
1	E	468	VAL
1	F	1	MET
1	F	13	VAL
1	F	55	THR
1	F	58	ASP
1	F	78	THR
1	F	82	THR
1	F	83	PHE
1	F	98	LYS
1	F	114	ASP
1	F	116	ILE
1	F	128	HIS
1	F	136	ILE
1	F	142	VAL
1	F	166	VAL
1	F	175	HIS
1	F	201	LYS
1	F	211	THR
1	F	252	ASN
1	F	285	LEU
1	F	287	GLN
1	F	332	ASP
1	F	347	SER
1	F	355	THR
1	F	370	ILE
1	F	374	ASP
1	F	380	VAL
1	F	382	THR

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Mol	Chain	Res	Type
1	F	394	SER
1	F	406	PRO
1	F	407	VAL
1	F	451	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	287	GLN
1	B	446	HIS
1	B	461	GLN
1	C	106	GLN
1	D	125	GLN
1	E	446	HIS
1	F	81	HIS
1	F	252	ASN
1	F	287	GLN
1	F	461	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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	474/474 (100%)	0.23	39 (8%)	14 9	29, 72, 143, 172	0
1	B	474/474 (100%)	0.01	18 (3%)	44 31	27, 57, 115, 221	0
1	C	474/474 (100%)	0.24	26 (5%)	29 18	35, 81, 134, 191	0
1	D	474/474 (100%)	0.38	40 (8%)	14 9	32, 83, 148, 204	0
1	E	474/474 (100%)	0.38	40 (8%)	14 9	33, 89, 151, 246	0
1	F	474/474 (100%)	0.29	37 (7%)	16 10	35, 78, 135, 165	0
All	All	2844/2844 (100%)	0.26	200 (7%)	19 12	27, 77, 140, 246	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	ASN	18.6
1	D	244	ASN	11.4
1	E	412	PRO	10.8
1	E	245	ASP	10.6
1	E	474	LYS	9.8
1	B	244	ASN	9.7
1	A	324	ASN	9.4
1	E	4	MET	8.8
1	E	411	THR	8.7
1	A	421	VAL	7.3
1	F	474	LYS	7.1
1	A	323	ASP	7.0
1	B	243	ASP	6.9
1	B	246	HIS	6.8
1	D	246	HIS	6.8
1	D	245	ASP	6.6
1	C	244	ASN	6.6
1	D	422	ALA	6.5
1	E	473	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
1	D	1	MET	6.0
1	A	242	GLY	5.9
1	D	372	GLY	5.7
1	B	1	MET	5.7
1	C	245	ASP	5.6
1	B	245	ASP	5.3
1	E	3	LYS	5.2
1	F	362	ARG	4.9
1	A	474	LYS	4.9
1	F	245	ASP	4.9
1	D	423	LYS	4.9
1	D	4	MET	4.9
1	C	47	PRO	4.8
1	E	413	GLU	4.8
1	E	234	GLU	4.8
1	D	107	PHE	4.7
1	A	243	ASP	4.7
1	E	246	HIS	4.7
1	A	288	LEU	4.6
1	B	242	GLY	4.5
1	A	371	GLY	4.4
1	C	414	ALA	4.4
1	A	244	ASN	4.4
1	D	2	ARG	4.3
1	F	49	GLU	4.3
1	E	262	GLY	4.3
1	D	243	ASP	4.3
1	F	244	ASN	4.3
1	D	363	VAL	4.3
1	B	325	LYS	4.2
1	F	242	GLY	4.2
1	A	123	LEU	4.2
1	D	325	LYS	4.2
1	D	5	GLN	4.2
1	B	365	VAL	4.2
1	F	4	MET	4.1
1	C	21	PRO	4.0
1	D	3	LYS	4.0
1	A	4	MET	4.0
1	A	261	LEU	4.0
1	B	432	LEU	3.9
1	D	290	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	326	GLN	3.9
1	A	369	GLY	3.8
1	A	367	PRO	3.8
1	C	473	ILE	3.8
1	D	324	ASN	3.8
1	E	244	ASN	3.8
1	F	291	LEU	3.8
1	D	118	MET	3.7
1	F	292	ALA	3.7
1	A	21	PRO	3.7
1	F	240	VAL	3.6
1	E	261	LEU	3.6
1	C	75	GLY	3.5
1	C	243	ASP	3.5
1	A	473	ILE	3.5
1	C	324	ASN	3.5
1	D	18	LEU	3.5
1	F	363	VAL	3.5
1	F	383	GLY	3.5
1	A	420	PRO	3.5
1	A	422	ALA	3.4
1	F	412	PRO	3.4
1	C	20	GLY	3.3
1	E	19	TYR	3.3
1	F	379	LEU	3.3
1	E	324	ASN	3.3
1	E	106	GLN	3.3
1	C	4	MET	3.3
1	D	413	GLU	3.3
1	D	404	GLY	3.2
1	F	368	LEU	3.2
1	C	365	VAL	3.2
1	B	454	LEU	3.2
1	A	368	LEU	3.2
1	C	240	VAL	3.1
1	A	241	GLU	3.1
1	A	414	ALA	3.1
1	F	118	MET	3.1
1	D	81	HIS	3.1
1	D	24	LEU	3.1
1	E	259	GLU	3.1
1	B	326	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	10	TRP	3.1
1	C	361	PRO	3.0
1	D	147	VAL	3.0
1	D	79	TRP	3.0
1	A	221	ILE	3.0
1	F	473	ILE	3.0
1	A	222	ALA	2.9
1	F	417	PRO	2.9
1	A	245	ASP	2.9
1	A	226	ILE	2.9
1	A	74	ALA	2.8
1	E	10	TRP	2.8
1	E	371	GLY	2.8
1	F	367	PRO	2.8
1	F	21	PRO	2.8
1	E	18	LEU	2.7
1	D	148	TYR	2.7
1	E	417	PRO	2.7
1	A	5	GLN	2.7
1	F	24	LEU	2.7
1	D	421	VAL	2.7
1	E	227	ASP	2.6
1	F	246	HIS	2.6
1	A	301	TYR	2.6
1	D	163	TRP	2.6
1	F	187	ASP	2.6
1	C	359	ASP	2.5
1	A	350	LEU	2.5
1	E	21	PRO	2.5
1	F	9	PHE	2.5
1	E	432	LEU	2.4
1	F	252	ASN	2.4
1	A	365	VAL	2.4
1	D	347	SER	2.4
1	A	325	LYS	2.4
1	F	388	GLY	2.4
1	D	151	TRP	2.4
1	F	419	LEU	2.4
1	D	7	TYR	2.4
1	C	45	ASP	2.4
1	F	243	ASP	2.4
1	F	374	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.4
1	A	24	LEU	2.4
1	C	372	GLY	2.3
1	F	241	GLU	2.3
1	E	27	VAL	2.3
1	A	372	GLY	2.3
1	E	407	VAL	2.3
1	D	146	SER	2.3
1	C	222	ALA	2.3
1	D	344	ILE	2.3
1	E	381	PHE	2.3
1	A	240	VAL	2.3
1	E	253	VAL	2.3
1	F	384	ALA	2.3
1	E	100	LEU	2.3
1	E	13	VAL	2.3
1	B	437	LYS	2.3
1	B	333	TYR	2.3
1	C	325	LYS	2.2
1	D	454	LEU	2.2
1	B	473	ILE	2.2
1	F	110	ASN	2.2
1	D	130	ASP	2.2
1	C	246	HIS	2.2
1	C	3	LYS	2.2
1	F	52	LEU	2.2
1	F	378	ARG	2.2
1	A	246	HIS	2.2
1	C	258	ARG	2.2
1	E	408	ASP	2.2
1	A	290	GLY	2.2
1	E	327	THR	2.2
1	E	304	GLY	2.2
1	C	2	ARG	2.2
1	D	343	ALA	2.2
1	D	103	LEU	2.2
1	B	7	TYR	2.2
1	A	252	ASN	2.1
1	E	5	GLN	2.1
1	A	280	GLN	2.1
1	E	24	LEU	2.1
1	E	314	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	227	ASP	2.1
1	E	392	THR	2.1
1	B	370	ILE	2.1
1	D	208	TYR	2.1
1	B	5	GLN	2.1
1	C	412	PRO	2.1
1	E	263	ILE	2.1
1	F	290	GLY	2.0
1	E	421	VAL	2.0
1	D	350	LEU	2.0
1	D	373	LYS	2.0
1	E	7	TYR	2.0
1	F	295	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.