



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:59 AM UTC

PDB ID : 1T8R / pdb_00001t8r
Title : Crystal Structure of E. coli AMP Nucleosidase
Authors : Zhang, Y.; Cottet, S.E.; Ealick, S.E.
Deposited on : 2004-05-13
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

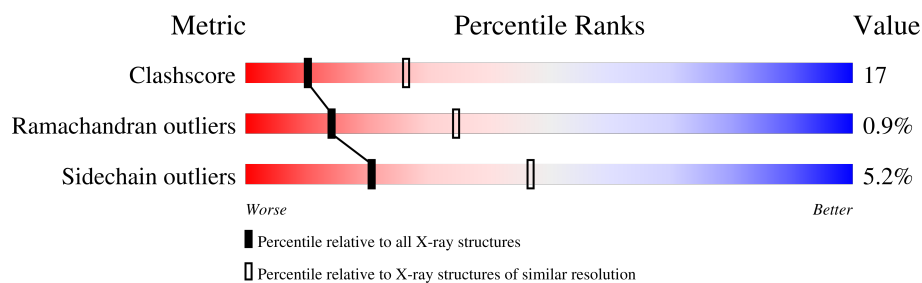
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	484	
1	B	484	
1	C	484	
1	D	484	
1	E	484	
1	F	484	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22181 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 AMP nucleosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	Se	0	0	0
			3662	2325	644	684	5	4			
1	B	463	Total	C	N	O	S	Se	0	0	0
			3662	2325	644	684	5	4			
1	C	463	Total	C	N	O	S	Se	0	0	0
			3662	2325	644	684	5	4			
1	D	463	Total	C	N	O	S	Se	0	0	0
			3662	2325	644	684	5	4			
1	E	463	Total	C	N	O	S	Se	0	0	0
			3662	2325	644	684	5	4			
1	F	463	Total	C	N	O	S	Se	0	0	0
			3662	2325	644	684	5	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MSE	MET	modified residue	UNP P15272
A	260	MSE	MET	modified residue	UNP P15272
A	302	MSE	MET	modified residue	UNP P15272
A	404	MSE	MET	modified residue	UNP P15272
B	138	MSE	MET	modified residue	UNP P15272
B	260	MSE	MET	modified residue	UNP P15272
B	302	MSE	MET	modified residue	UNP P15272
B	404	MSE	MET	modified residue	UNP P15272
C	138	MSE	MET	modified residue	UNP P15272
C	260	MSE	MET	modified residue	UNP P15272
C	302	MSE	MET	modified residue	UNP P15272
C	404	MSE	MET	modified residue	UNP P15272
D	138	MSE	MET	modified residue	UNP P15272
D	260	MSE	MET	modified residue	UNP P15272
D	302	MSE	MET	modified residue	UNP P15272
D	404	MSE	MET	modified residue	UNP P15272
E	138	MSE	MET	modified residue	UNP P15272

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Chain	Residue	Modelled	Actual	Comment	Reference
E	260	MSE	MET	modified residue	UNP P15272
E	302	MSE	MET	modified residue	UNP P15272
E	404	MSE	MET	modified residue	UNP P15272
F	138	MSE	MET	modified residue	UNP P15272
F	260	MSE	MET	modified residue	UNP P15272
F	302	MSE	MET	modified residue	UNP P15272
F	404	MSE	MET	modified residue	UNP P15272

- Molecule 2 is water.

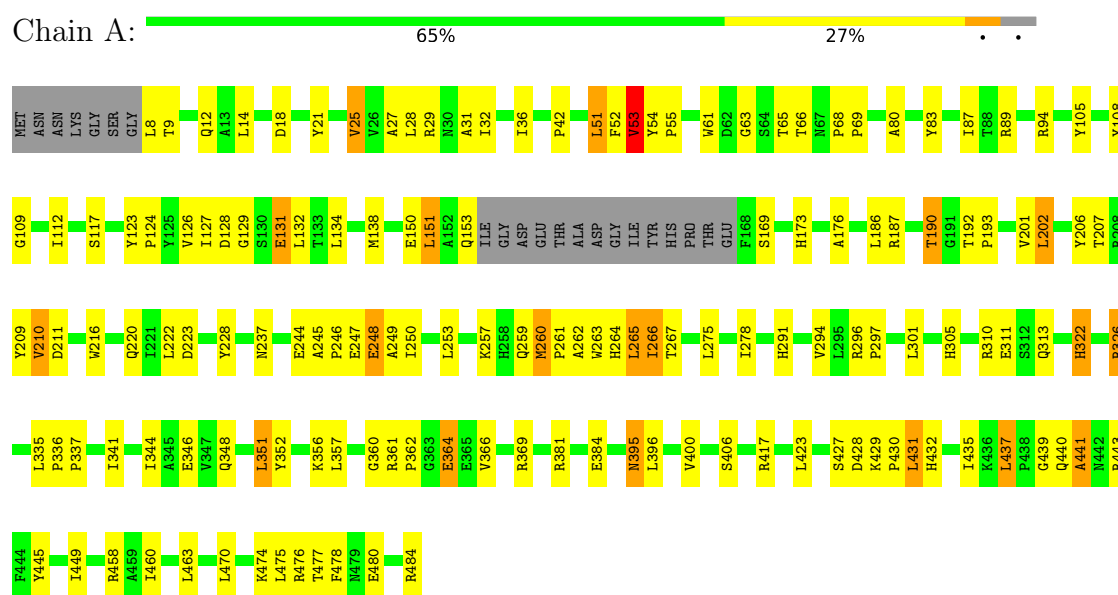
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	33	Total O 33 33	0	0
2	B	39	Total O 39 39	0	0
2	C	37	Total O 37 37	0	0
2	D	40	Total O 40 40	0	0
2	E	35	Total O 35 35	0	0
2	F	25	Total O 25 25	0	0

3 Residue-property plots

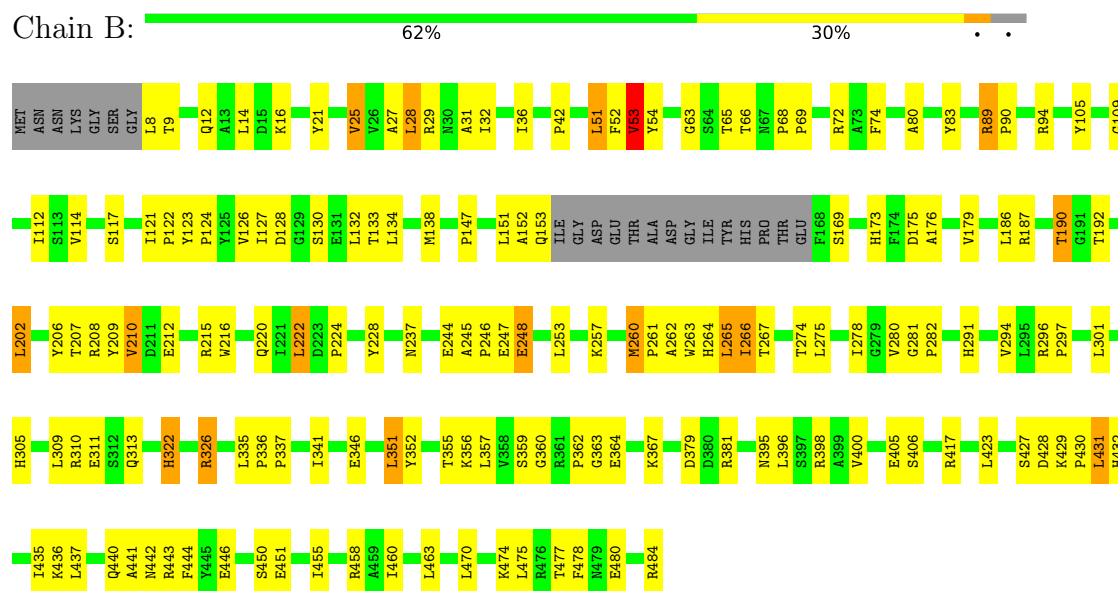
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

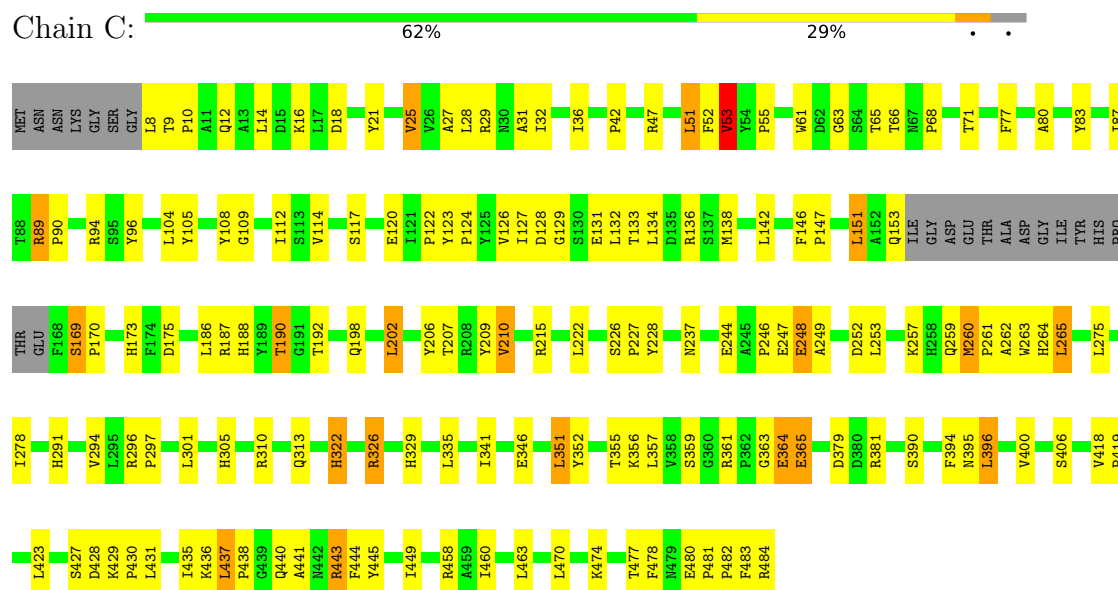
• Molecule 1: AMP nucleosidase



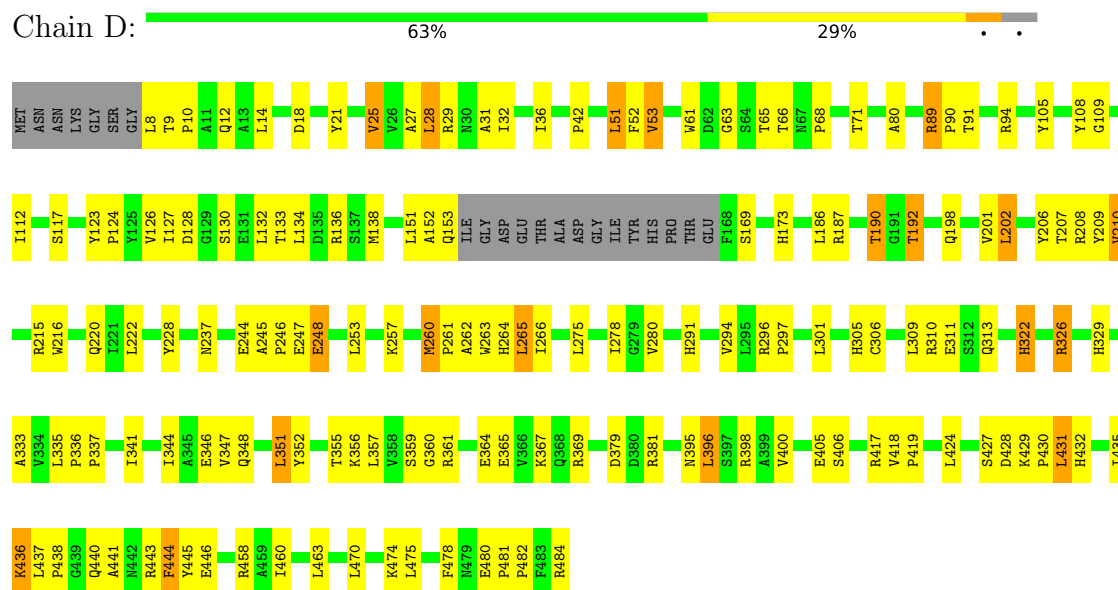
• Molecule 1: AMP nucleosidase



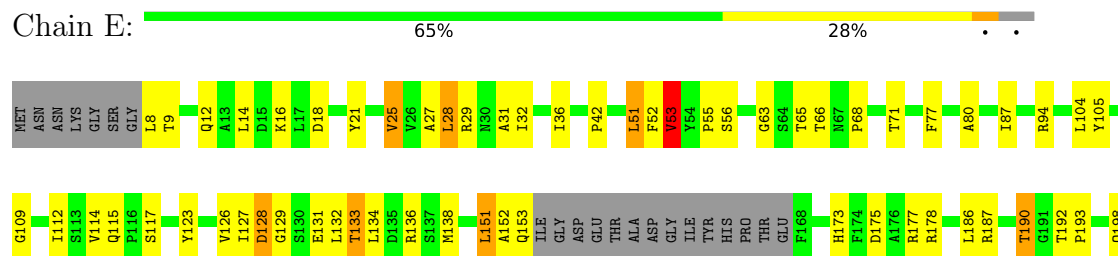
• Molecule 1: AMP nucleosidase

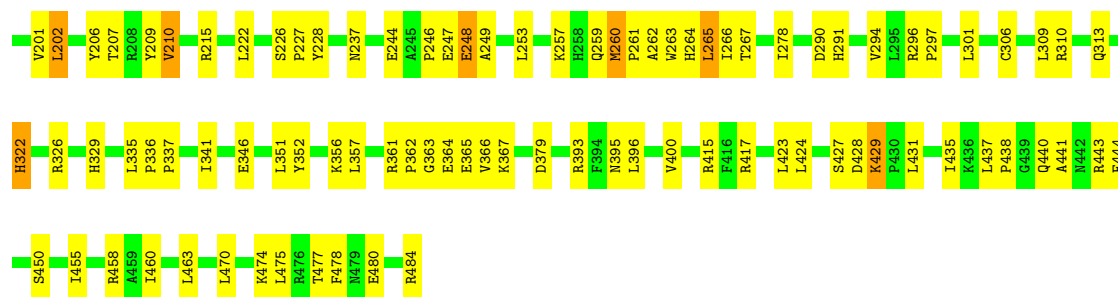


• Molecule 1: AMP nucleosidase



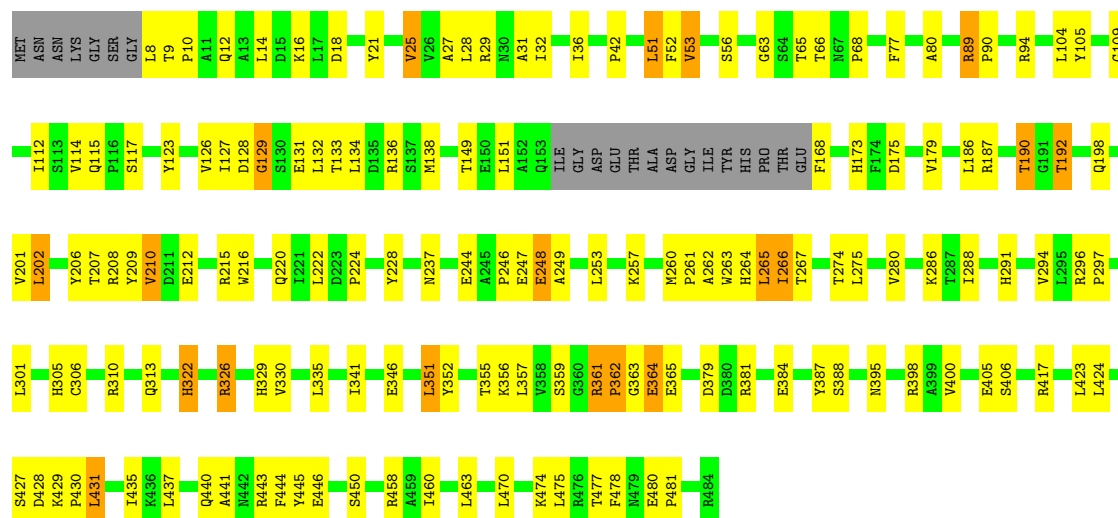
• Molecule 1: AMP nucleosidase





• Molecule 1: AMP nucleosidase

Chain F: 63% 29%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	246.63Å 246.63Å 111.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.22 – 2.70	Depositor
% Data completeness (in resolution range)	95.7 (25.22-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22181	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/3752	0.93	9/5107 (0.2%)
1	B	0.48	0/3752	0.94	9/5107 (0.2%)
1	C	0.49	0/3752	0.94	13/5107 (0.3%)
1	D	0.51	0/3752	0.94	11/5107 (0.2%)
1	E	0.49	0/3752	0.92	9/5107 (0.2%)
1	F	0.46	0/3752	0.94	12/5107 (0.2%)
All	All	0.49	0/22512	0.94	63/30642 (0.2%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	429	LYS	CA-C-N	8.37	127.94	119.24
1	F	429	LYS	C-N-CA	8.37	127.94	119.24
1	B	53	VAL	N-CA-C	7.46	119.82	108.71
1	A	53	VAL	N-CA-C	7.31	119.60	108.71
1	F	53	VAL	N-CA-C	7.23	119.49	108.71
1	D	260	MSE	CA-C-N	7.10	127.14	119.90
1	D	260	MSE	C-N-CA	7.10	127.14	119.90
1	F	260	MSE	CA-C-N	7.09	127.13	119.90
1	F	260	MSE	C-N-CA	7.09	127.13	119.90
1	D	53	VAL	N-CA-C	7.09	119.27	108.71
1	E	429	LYS	CA-C-N	7.06	127.37	119.32
1	E	429	LYS	C-N-CA	7.06	127.37	119.32
1	B	429	LYS	CA-C-N	6.95	127.24	119.32
1	B	429	LYS	C-N-CA	6.95	127.24	119.32
1	E	53	VAL	N-CA-C	6.95	119.06	108.71
1	C	429	LYS	CA-C-N	6.92	127.21	119.32
1	C	429	LYS	C-N-CA	6.92	127.21	119.32
1	A	429	LYS	CA-C-N	6.89	127.17	119.32
1	A	429	LYS	C-N-CA	6.89	127.17	119.32
1	A	260	MSE	CA-C-N	6.73	126.76	119.90
1	A	260	MSE	C-N-CA	6.73	126.76	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	361	ARG	CA-C-N	6.66	128.17	119.84
1	F	361	ARG	C-N-CA	6.66	128.17	119.84
1	D	429	LYS	CA-C-N	6.61	126.85	119.32
1	D	429	LYS	C-N-CA	6.61	126.85	119.32
1	A	439	GLY	N-CA-C	-6.53	106.71	114.48
1	C	53	VAL	N-CA-C	6.40	118.25	108.71
1	C	260	MSE	CA-C-N	6.33	126.36	119.90
1	C	260	MSE	C-N-CA	6.33	126.36	119.90
1	B	260	MSE	CA-C-N	6.32	126.35	119.90
1	B	260	MSE	C-N-CA	6.32	126.35	119.90
1	C	449	ILE	N-CA-C	6.30	116.98	110.36
1	D	201	VAL	N-CA-C	6.14	117.86	108.71
1	C	198	GLN	CA-C-N	6.13	125.76	119.56
1	C	198	GLN	C-N-CA	6.13	125.76	119.56
1	A	449	ILE	N-CA-C	6.08	117.56	110.62
1	C	443	ARG	N-CA-C	5.90	117.72	111.28
1	E	260	MSE	CA-C-N	5.73	125.74	119.90
1	E	260	MSE	C-N-CA	5.73	125.74	119.90
1	B	326	ARG	N-CA-C	5.71	118.73	108.17
1	E	128	ASP	N-CA-C	5.70	117.98	111.02
1	D	198	GLN	CA-C-N	5.64	125.32	119.56
1	D	198	GLN	C-N-CA	5.64	125.32	119.56
1	F	201	VAL	N-CA-C	5.49	116.49	108.53
1	C	365	GLU	N-CA-C	-5.48	105.47	111.82
1	F	326	ARG	N-CA-C	5.43	118.21	108.17
1	D	326	ARG	N-CA-C	5.34	118.04	108.17
1	C	326	ARG	N-CA-C	5.32	118.00	108.17
1	A	326	ARG	N-CA-C	5.24	117.86	108.17
1	B	266	ILE	N-CA-C	5.23	117.38	109.12
1	A	266	ILE	N-CA-C	5.17	117.29	109.12
1	F	266	ILE	N-CA-C	5.14	117.24	109.12
1	C	169	SER	CA-C-N	5.08	125.32	119.83
1	C	169	SER	C-N-CA	5.08	125.32	119.83
1	E	201	VAL	N-CA-C	5.05	115.86	108.53
1	B	379	ASP	N-CA-C	-5.05	106.71	112.92
1	B	444	PHE	N-CA-C	5.05	119.29	113.18
1	D	444	PHE	N-CA-C	5.04	119.14	112.89
1	D	266	ILE	N-CA-C	5.03	117.06	109.12
1	F	198	GLN	CA-C-N	5.02	124.63	119.56
1	F	198	GLN	C-N-CA	5.02	124.63	119.56
1	E	198	GLN	CA-C-N	5.02	124.81	119.28
1	E	198	GLN	C-N-CA	5.02	124.81	119.28

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	3662	0	3589	133	0
1	B	3662	0	3589	139	0
1	C	3662	0	3589	145	0
1	D	3662	0	3589	139	0
1	E	3662	0	3589	135	0
1	F	3662	0	3589	135	0
2	A	33	0	0	0	0
2	B	39	0	0	1	0
2	C	37	0	0	0	0
2	D	40	0	0	3	0
2	E	35	0	0	3	0
2	F	25	0	0	1	0
All	All	22181	0	21534	742	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 17.

All (742) 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:A:190:THR:CG2	1:A:192:THR:HB	1.84	1.07
1:E:131:GLU:HB2	1:F:441:ALA:HB3	1.36	1.04
1:D:190:THR:CG2	1:D:192:THR:HB	1.87	1.04
1:A:151:LEU:H	1:A:151:LEU:HD22	1.22	1.02
1:A:192:THR:HG21	1:A:264:HIS:NE2	1.73	1.02
1:C:190:THR:CG2	1:C:192:THR:HB	1.90	1.02
1:D:190:THR:HG22	1:D:192:THR:HB	1.41	1.02
1:D:192:THR:HG21	1:D:264:HIS:NE2	1.74	1.01
1:B:190:THR:CG2	1:B:192:THR:HB	1.91	1.00
1:C:192:THR:HG21	1:C:264:HIS:NE2	1.77	0.99
1:F:192:THR:HG21	1:F:264:HIS:NE2	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:THR:CG2	1:E:192:THR:HB	1.95	0.97
1:E:192:THR:HG21	1:E:264:HIS:NE2	1.79	0.97
1:F:190:THR:HG22	1:F:192:THR:HB	1.42	0.97
1:C:190:THR:HG22	1:C:192:THR:HB	1.42	0.97
1:E:190:THR:HG22	1:E:192:THR:HB	1.47	0.96
1:F:361:ARG:HB3	1:F:365:GLU:HB2	1.46	0.96
1:B:190:THR:HG22	1:B:192:THR:HB	1.47	0.95
1:F:190:THR:CG2	1:F:192:THR:HB	1.95	0.95
1:A:190:THR:HG22	1:A:192:THR:HB	1.49	0.94
1:E:441:ALA:HB3	1:F:131:GLU:HB2	1.47	0.94
1:B:192:THR:HG21	1:B:264:HIS:NE2	1.82	0.94
1:E:361:ARG:HB3	1:E:365:GLU:HB2	1.53	0.89
1:E:202:LEU:HD13	1:E:460:ILE:HD11	1.56	0.87
1:F:310:ARG:H	1:F:313:GLN:HE21	1.19	0.87
1:C:443:ARG:HE	1:D:133:THR:HG23	1.40	0.86
1:A:202:LEU:HD13	1:A:460:ILE:HD11	1.57	0.85
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.41	0.84
1:E:310:ARG:H	1:E:313:GLN:HE21	1.26	0.84
1:C:202:LEU:HD13	1:C:460:ILE:HD11	1.60	0.83
1:F:190:THR:HG23	1:F:262:ALA:HB3	1.58	0.82
1:F:202:LEU:HD13	1:F:460:ILE:HD11	1.62	0.82
1:A:395:ASN:HD21	1:F:477:THR:HB	1.44	0.82
1:E:443:ARG:HE	1:F:133:THR:HG22	1.43	0.82
1:C:431:LEU:HD12	1:D:151:LEU:HD22	1.62	0.81
1:C:36:ILE:HG23	1:C:138:MSE:HE1	1.61	0.81
1:D:202:LEU:HD13	1:D:460:ILE:HD11	1.62	0.80
1:B:202:LEU:HD13	1:B:460:ILE:HD11	1.64	0.80
1:A:186:LEU:O	1:A:190:THR:HB	1.81	0.80
1:E:435:ILE:HD11	1:F:151:LEU:HD11	1.63	0.80
1:F:127:ILE:HD13	1:F:132:LEU:HG	1.62	0.79
1:F:310:ARG:H	1:F:313:GLN:NE2	1.81	0.78
1:D:361:ARG:HB3	1:D:364:GLU:HG2	1.65	0.78
1:B:65:THR:HB	1:B:68:PRO:HG3	1.66	0.77
1:E:310:ARG:H	1:E:313:GLN:NE2	1.81	0.77
1:C:430:PRO:HA	1:C:435:ILE:HG12	1.66	0.76
1:F:326:ARG:HG2	1:F:326:ARG:HH11	1.50	0.76
1:B:478:PHE:HD1	1:C:395:ASN:HD22	1.34	0.75
1:B:360:GLY:O	1:B:362:PRO:HD3	1.87	0.75
1:C:190:THR:HG23	1:C:262:ALA:HB3	1.67	0.75
1:E:190:THR:HG23	1:E:262:ALA:HB3	1.68	0.75
1:C:127:ILE:HD13	1:C:132:LEU:HG	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ARG:HG2	1:B:326:ARG:HH11	1.52	0.74
1:D:134:LEU:HD23	1:D:138:MSE:HB3	1.67	0.74
1:D:186:LEU:O	1:D:190:THR:HB	1.88	0.74
1:F:361:ARG:H	1:F:361:ARG:HD3	1.53	0.74
1:B:186:LEU:O	1:B:190:THR:HB	1.87	0.74
1:B:478:PHE:H	1:C:395:ASN:HD21	1.36	0.73
1:D:36:ILE:HD11	1:D:132:LEU:HD13	1.70	0.73
1:B:134:LEU:HD23	1:B:138:MSE:HB3	1.69	0.73
1:B:190:THR:HG23	1:B:262:ALA:HB3	1.70	0.73
1:D:326:ARG:HG2	1:D:326:ARG:HH11	1.53	0.73
1:E:186:LEU:O	1:E:190:THR:HB	1.88	0.72
1:C:65:THR:HB	1:C:68:PRO:HG3	1.71	0.72
1:E:361:ARG:HG2	1:E:365:GLU:OE1	1.89	0.72
1:F:207:THR:O	1:F:210:VAL:HG13	1.89	0.72
1:D:190:THR:HG23	1:D:262:ALA:HB3	1.72	0.72
1:C:326:ARG:HH11	1:C:326:ARG:HG2	1.55	0.71
1:E:437:LEU:HD12	1:E:440:GLN:OE1	1.90	0.71
1:E:326:ARG:HH11	1:E:326:ARG:HG2	1.56	0.71
1:C:310:ARG:H	1:C:313:GLN:NE2	1.89	0.70
1:A:127:ILE:HD13	1:A:132:LEU:HG	1.73	0.70
1:C:186:LEU:O	1:C:190:THR:HB	1.91	0.70
1:F:437:LEU:HD12	1:F:440:GLN:OE1	1.91	0.70
1:F:186:LEU:O	1:F:190:THR:HB	1.92	0.69
1:A:384:GLU:HB3	1:B:151:LEU:HD11	1.75	0.69
1:D:228:TYR:CG	1:D:265:LEU:HD13	2.26	0.69
1:F:65:THR:HB	1:F:68:PRO:HG3	1.72	0.69
1:D:51:LEU:HD13	1:D:52:PHE:CE2	2.28	0.69
1:E:207:THR:O	1:E:210:VAL:HG13	1.93	0.69
1:E:133:THR:HG22	1:F:443:ARG:HB2	1.75	0.69
1:D:32:ILE:HD11	1:D:123:TYR:HB2	1.73	0.68
1:E:32:ILE:HD11	1:E:123:TYR:HB2	1.74	0.68
1:E:65:THR:HB	1:E:68:PRO:HG3	1.75	0.68
1:F:32:ILE:HD11	1:F:123:TYR:HB2	1.75	0.68
1:A:395:ASN:ND2	1:F:477:THR:HB	2.08	0.68
1:E:192:THR:HG21	1:E:264:HIS:CD2	2.29	0.68
1:E:134:LEU:HD23	1:E:138:MSE:HB3	1.74	0.68
1:E:187:ARG:HG3	1:E:187:ARG:HH11	1.58	0.67
1:B:437:LEU:HD12	1:B:440:GLN:OE1	1.94	0.67
1:A:36:ILE:HG23	1:A:138:MSE:HE1	1.75	0.67
1:B:395:ASN:HD21	1:C:477:THR:HB	1.59	0.67
1:B:36:ILE:HG23	1:B:138:MSE:HE1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ARG:HH11	1:C:187:ARG:HG3	1.59	0.67
1:C:329:HIS:HD2	1:C:379:ASP:OD2	1.78	0.67
1:D:395:ASN:HD21	1:E:477:THR:HB	1.59	0.67
1:F:36:ILE:HG23	1:F:138:MSE:HE1	1.76	0.67
1:D:65:THR:HB	1:D:68:PRO:HG3	1.77	0.67
1:A:360:GLY:O	1:A:362:PRO:HD3	1.95	0.67
1:A:477:THR:HB	1:F:395:ASN:HD21	1.60	0.66
1:A:187:ARG:HG3	1:A:187:ARG:HH11	1.61	0.66
1:A:430:PRO:HA	1:A:435:ILE:HG12	1.77	0.66
1:F:134:LEU:HD23	1:F:138:MSE:HB3	1.76	0.66
1:E:21:TYR:O	1:E:25:VAL:HG12	1.94	0.66
1:A:207:THR:O	1:A:210:VAL:HG13	1.95	0.66
1:C:207:THR:O	1:C:210:VAL:HG13	1.97	0.65
1:D:36:ILE:CD1	1:D:132:LEU:HD13	2.26	0.65
1:A:134:LEU:HD23	1:A:138:MSE:HB3	1.77	0.65
1:B:478:PHE:H	1:C:395:ASN:ND2	1.93	0.65
1:D:395:ASN:ND2	1:E:478:PHE:H	1.95	0.65
1:C:310:ARG:H	1:C:313:GLN:HE21	1.43	0.65
1:E:132:LEU:HB3	1:E:134:LEU:CD1	2.26	0.65
1:F:192:THR:HG21	1:F:264:HIS:CD2	2.31	0.65
1:C:32:ILE:HD11	1:C:123:TYR:HB2	1.79	0.64
1:D:187:ARG:HG3	1:D:187:ARG:HH11	1.62	0.64
1:B:187:ARG:HG3	1:B:187:ARG:HH11	1.63	0.64
1:B:228:TYR:CG	1:B:265:LEU:HD13	2.31	0.64
1:C:352:TYR:CE2	1:C:356:LYS:HE3	2.32	0.64
1:A:65:THR:HB	1:A:68:PRO:HG3	1.79	0.64
1:A:151:LEU:H	1:A:151:LEU:CD2	2.01	0.64
1:B:207:THR:O	1:B:210:VAL:HG13	1.97	0.64
1:D:9:THR:OG1	1:D:12:GLN:HG3	1.98	0.64
1:D:21:TYR:O	1:D:25:VAL:HG12	1.98	0.64
1:F:27:ALA:HB1	1:F:51:LEU:HD22	1.79	0.64
1:C:192:THR:HG21	1:C:264:HIS:CD2	2.32	0.63
1:C:435:ILE:HD11	1:D:151:LEU:HD11	1.79	0.63
1:D:244:GLU:O	1:D:246:PRO:HD3	1.98	0.63
1:D:310:ARG:H	1:D:313:GLN:NE2	1.96	0.63
1:B:192:THR:HG21	1:B:264:HIS:CD2	2.33	0.63
1:F:132:LEU:HB3	1:F:134:LEU:HD13	1.79	0.63
1:B:9:THR:OG1	1:B:12:GLN:HG3	1.99	0.63
1:C:151:LEU:CD2	1:D:431:LEU:HD12	2.28	0.63
1:C:443:ARG:HE	1:D:133:THR:CG2	2.09	0.63
1:D:237:ASN:HD21	1:D:248:GLU:HB3	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LEU:HD21	1:C:257:LYS:HE3	1.81	0.62
1:D:322:HIS:HD2	1:E:474:LYS:HD3	1.63	0.62
1:E:27:ALA:HB1	1:E:51:LEU:HD22	1.79	0.62
1:E:51:LEU:HD13	1:E:52:PHE:CE2	2.34	0.62
1:A:326:ARG:HG2	1:A:326:ARG:NH1	2.11	0.62
1:A:131:GLU:HB2	1:B:441:ALA:HB3	1.82	0.62
1:E:36:ILE:HG23	1:E:138:MSE:HE1	1.82	0.62
1:B:237:ASN:HD21	1:B:248:GLU:HB3	1.65	0.62
1:E:29:ARG:NH2	1:E:128:ASP:HB2	2.15	0.62
1:B:360:GLY:C	1:B:362:PRO:HD3	2.24	0.62
1:A:395:ASN:ND2	1:F:478:PHE:H	1.98	0.62
1:D:335:LEU:HD21	1:D:341:ILE:HD11	1.81	0.62
1:A:131:GLU:CD	1:A:131:GLU:H	2.07	0.62
1:A:192:THR:HG21	1:A:264:HIS:CD2	2.34	0.61
1:B:132:LEU:O	1:B:134:LEU:HD12	2.00	0.61
1:B:310:ARG:H	1:B:313:GLN:NE2	1.97	0.61
1:D:367:LYS:HB3	1:E:71:THR:CG2	2.30	0.61
1:B:32:ILE:HD11	1:B:123:TYR:HB2	1.81	0.61
1:A:190:THR:HG23	1:A:262:ALA:HB3	1.83	0.61
1:E:335:LEU:HD21	1:E:341:ILE:HD11	1.83	0.61
1:F:253:LEU:HD21	1:F:257:LYS:HE3	1.83	0.61
1:D:27:ALA:HB1	1:D:51:LEU:HD22	1.81	0.61
1:A:440:GLN:HE21	1:A:440:GLN:HA	1.66	0.60
1:C:151:LEU:HD23	1:D:431:LEU:HD12	1.84	0.60
1:C:134:LEU:HD23	1:C:138:MSE:HB3	1.83	0.60
1:E:244:GLU:O	1:E:246:PRO:HD3	2.01	0.60
1:B:127:ILE:HG22	1:B:130:SER:H	1.67	0.60
1:C:131:GLU:HB2	1:D:441:ALA:HB3	1.84	0.60
1:A:151:LEU:HD21	1:B:431:LEU:HA	1.83	0.60
1:F:53:VAL:HG11	1:F:117:SER:O	2.01	0.60
1:A:435:ILE:HD11	1:B:151:LEU:HD13	1.84	0.59
1:B:352:TYR:CE2	1:B:356:LYS:HE3	2.37	0.59
1:F:14:LEU:HD13	1:F:94:ARG:HD3	1.84	0.59
1:C:9:THR:HG23	1:C:12:GLN:HE21	1.66	0.59
1:A:253:LEU:HD21	1:A:257:LYS:HE3	1.83	0.59
1:E:127:ILE:HG22	1:E:127:ILE:O	2.00	0.59
1:A:244:GLU:O	1:A:246:PRO:HD3	2.03	0.59
1:A:9:THR:OG1	1:A:12:GLN:HG3	2.02	0.59
1:A:27:ALA:HB1	1:A:51:LEU:HD22	1.83	0.59
1:D:132:LEU:HB2	1:D:134:LEU:HD11	1.84	0.59
1:F:187:ARG:HG3	1:F:187:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:PHE:HD1	1:C:395:ASN:ND2	2.01	0.59
1:E:352:TYR:CE2	1:E:356:LYS:HE3	2.38	0.59
1:C:244:GLU:O	1:C:246:PRO:HD3	2.02	0.59
1:C:305:HIS:CE1	1:C:438:PRO:HG2	2.37	0.59
1:C:63:GLY:HA3	1:C:80:ALA:HB2	1.85	0.59
1:D:253:LEU:HD21	1:D:257:LYS:HE3	1.84	0.59
1:F:29:ARG:NH2	1:F:128:ASP:HB2	2.17	0.59
1:F:224:PRO:HA	2:F:493:HOH:O	2.02	0.59
1:D:395:ASN:HD21	1:E:478:PHE:H	1.51	0.58
1:E:63:GLY:HA3	1:E:80:ALA:HB2	1.85	0.58
1:D:9:THR:HG23	1:D:12:GLN:HE21	1.68	0.58
1:D:132:LEU:HB2	1:D:134:LEU:CD1	2.33	0.58
1:B:127:ILE:CG2	1:B:130:SER:HA	2.34	0.58
1:E:14:LEU:HD13	1:E:94:ARG:HD3	1.84	0.58
1:E:253:LEU:HD21	1:E:257:LYS:HE3	1.85	0.58
1:B:27:ALA:HB1	1:B:51:LEU:HD22	1.86	0.58
1:B:322:HIS:HD2	1:C:474:LYS:HD3	1.69	0.58
1:C:259:GLN:OE1	1:D:381:ARG:NH2	2.32	0.58
1:A:310:ARG:H	1:A:313:GLN:NE2	2.02	0.58
1:E:363:GLY:O	1:E:366:VAL:HG22	2.03	0.58
1:A:478:PHE:H	1:F:395:ASN:ND2	2.01	0.58
1:B:63:GLY:HA3	1:B:80:ALA:HB2	1.85	0.58
1:A:32:ILE:HD11	1:A:123:TYR:HB2	1.86	0.58
1:D:329:HIS:HD2	1:D:379:ASP:OD2	1.87	0.58
1:F:9:THR:HG23	1:F:12:GLN:HE21	1.67	0.58
1:B:83:TYR:HA	1:B:169:SER:O	2.04	0.57
1:D:395:ASN:ND2	1:E:477:THR:HB	2.19	0.57
1:A:335:LEU:HD21	1:A:341:ILE:HD11	1.86	0.57
1:D:36:ILE:HG23	1:D:138:MSE:HE1	1.85	0.57
1:F:9:THR:OG1	1:F:12:GLN:HG3	2.04	0.57
1:D:228:TYR:CD1	1:D:265:LEU:HD13	2.40	0.57
1:E:177:ARG:HG3	2:E:485:HOH:O	2.03	0.57
1:F:132:LEU:HB3	1:F:134:LEU:CD1	2.35	0.57
1:F:208:ARG:HD3	1:F:446:GLU:OE1	2.05	0.57
1:E:361:ARG:HH11	1:E:361:ARG:HG3	1.69	0.57
1:A:151:LEU:HD22	1:A:151:LEU:N	2.07	0.57
1:A:478:PHE:H	1:F:395:ASN:HD21	1.52	0.57
1:E:9:THR:OG1	1:E:12:GLN:HG3	2.03	0.57
1:B:51:LEU:HD13	1:B:52:PHE:CE2	2.40	0.57
1:C:27:ALA:HB1	1:C:51:LEU:HD22	1.86	0.57
1:D:192:THR:HG21	1:D:264:HIS:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:THR:O	1:D:359:SER:HB3	2.05	0.57
1:B:36:ILE:HG23	1:B:138:MSE:CE	2.35	0.57
1:F:63:GLY:HA3	1:F:80:ALA:HB2	1.87	0.57
1:D:207:THR:O	1:D:210:VAL:HG13	2.04	0.56
1:E:187:ARG:HG3	1:E:187:ARG:NH1	2.20	0.56
1:E:443:ARG:NE	1:F:133:THR:HG22	2.15	0.56
1:C:9:THR:OG1	1:C:12:GLN:HG3	2.06	0.56
1:D:63:GLY:HA3	1:D:80:ALA:HB2	1.86	0.56
1:C:36:ILE:HG23	1:C:138:MSE:CE	2.34	0.56
1:A:395:ASN:HD21	1:F:478:PHE:H	1.53	0.56
1:B:173:HIS:HE1	1:B:480:GLU:OE2	1.88	0.56
1:E:237:ASN:HD21	1:E:248:GLU:HB3	1.71	0.56
1:B:395:ASN:ND2	1:C:477:THR:HB	2.19	0.56
1:B:127:ILE:HG22	1:B:130:SER:N	2.21	0.56
1:D:14:LEU:HD13	1:D:94:ARG:HD3	1.88	0.56
1:B:151:LEU:C	1:B:153:GLN:H	2.13	0.56
1:D:208:ARG:HD3	1:D:446:GLU:OE1	2.06	0.56
1:A:63:GLY:HA3	1:A:80:ALA:HB2	1.88	0.56
1:C:356:LYS:HE2	1:C:363:GLY:O	2.06	0.56
1:F:237:ASN:HD21	1:F:248:GLU:HB3	1.70	0.56
1:F:326:ARG:HG2	1:F:326:ARG:NH1	2.19	0.56
1:A:132:LEU:HB3	1:A:134:LEU:CD1	2.36	0.55
1:F:244:GLU:O	1:F:246:PRO:HD3	2.04	0.55
1:B:187:ARG:HG3	1:B:187:ARG:NH1	2.22	0.55
1:B:335:LEU:HD21	1:B:341:ILE:HD11	1.89	0.55
1:D:215:ARG:HG2	1:D:215:ARG:HH11	1.71	0.55
1:B:367:LYS:HB3	1:C:71:THR:HG23	1.88	0.55
1:C:51:LEU:HD13	1:C:52:PHE:CE2	2.42	0.55
1:D:187:ARG:HG3	1:D:187:ARG:NH1	2.22	0.55
1:A:427:SER:O	1:A:428:ASP:HB3	2.07	0.55
1:E:9:THR:HG23	1:E:12:GLN:HE21	1.71	0.55
1:E:291:HIS:O	1:E:294:VAL:HG22	2.06	0.55
1:D:29:ARG:NH2	1:D:128:ASP:HB2	2.21	0.54
1:A:127:ILE:O	1:A:127:ILE:HG22	2.06	0.54
1:B:253:LEU:HD21	1:B:257:LYS:HE3	1.89	0.54
1:B:367:LYS:HB3	1:C:71:THR:CG2	2.36	0.54
1:C:83:TYR:HA	1:C:169:SER:O	2.07	0.54
1:E:8:LEU:HB3	1:E:112:ILE:O	2.08	0.54
1:B:237:ASN:ND2	1:B:248:GLU:HB3	2.22	0.54
1:C:127:ILE:HG22	1:C:127:ILE:O	2.07	0.54
1:E:228:TYR:CG	1:E:265:LEU:HD13	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:LEU:HD12	1:D:151:LEU:CD2	2.35	0.54
1:F:77:PHE:CE2	1:F:104:LEU:HD22	2.43	0.54
1:A:417:ARG:HA	1:A:475:LEU:HD13	1.89	0.54
1:B:14:LEU:HD13	1:B:94:ARG:HD3	1.89	0.54
1:D:53:VAL:HG11	1:D:117:SER:O	2.07	0.54
1:B:311:GLU:HB3	1:B:432:HIS:NE2	2.23	0.54
1:E:173:HIS:HE1	1:E:480:GLU:OE2	1.90	0.54
1:B:21:TYR:O	1:B:25:VAL:HG12	2.07	0.53
1:B:296:ARG:HD3	1:B:484:ARG:OXT	2.08	0.53
1:C:190:THR:HG22	1:C:192:THR:CB	2.29	0.53
1:D:463:LEU:HD22	1:D:470:LEU:HD13	1.90	0.53
1:B:9:THR:HG23	1:B:12:GLN:HE21	1.73	0.53
1:C:175:ASP:OD1	1:C:175:ASP:C	2.50	0.53
1:A:237:ASN:HD21	1:A:248:GLU:HB3	1.73	0.53
1:C:275:LEU:C	1:C:275:LEU:HD23	2.34	0.53
1:D:153:GLN:NE2	2:D:494:HOH:O	2.41	0.53
1:F:228:TYR:HB3	1:F:265:LEU:HD22	1.90	0.53
1:B:244:GLU:O	1:B:246:PRO:HD3	2.08	0.53
1:E:415:ARG:HD2	2:E:510:HOH:O	2.09	0.53
1:D:28:LEU:HD13	1:D:126:VAL:HG21	1.91	0.53
1:D:322:HIS:CD2	1:E:474:LYS:HD3	2.42	0.53
1:D:381:ARG:HG3	1:D:381:ARG:O	2.08	0.53
1:C:132:LEU:HB3	1:C:134:LEU:HD13	1.90	0.53
1:F:329:HIS:HD2	1:F:379:ASP:OD2	1.91	0.53
1:B:36:ILE:HA	1:B:138:MSE:HE1	1.89	0.53
1:C:326:ARG:HG2	1:C:326:ARG:NH1	2.23	0.53
1:A:134:LEU:HD23	1:A:138:MSE:HE3	1.91	0.52
1:B:346:GLU:CD	1:B:346:GLU:H	2.17	0.52
1:E:151:LEU:O	1:E:153:GLN:HG2	2.09	0.52
1:B:395:ASN:ND2	1:C:478:PHE:H	2.07	0.52
1:F:36:ILE:HG23	1:F:138:MSE:CE	2.38	0.52
1:F:352:TYR:CE2	1:F:356:LYS:HE3	2.43	0.52
1:D:367:LYS:HB3	1:E:71:THR:HG23	1.90	0.52
1:C:355:THR:O	1:C:359:SER:HB3	2.08	0.52
1:C:187:ARG:HG3	1:C:187:ARG:NH1	2.20	0.52
1:A:202:LEU:HD13	1:A:460:ILE:CD1	2.35	0.52
1:B:8:LEU:HB3	1:B:112:ILE:O	2.09	0.52
1:B:208:ARG:HD3	1:B:446:GLU:OE1	2.09	0.52
1:E:463:LEU:HD22	1:E:470:LEU:HD13	1.92	0.52
1:C:435:ILE:HD11	1:D:151:LEU:CD1	2.40	0.52
1:A:83:TYR:HA	1:A:169:SER:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:362:PRO:HD2	1:F:365:GLU:OE1	2.10	0.52
1:A:310:ARG:H	1:A:313:GLN:HE21	1.56	0.51
1:B:291:HIS:O	1:B:294:VAL:HG22	2.10	0.51
1:C:29:ARG:NH2	1:C:128:ASP:HB2	2.25	0.51
1:D:215:ARG:HG2	1:D:215:ARG:NH1	2.24	0.51
1:A:477:THR:HB	1:F:395:ASN:ND2	2.24	0.51
1:E:131:GLU:CB	1:F:441:ALA:HB3	2.24	0.51
1:E:326:ARG:HG2	1:E:326:ARG:NH1	2.24	0.51
1:F:228:TYR:CG	1:F:265:LEU:HD13	2.46	0.51
1:D:326:ARG:HG2	1:D:326:ARG:NH1	2.21	0.51
1:F:134:LEU:N	1:F:134:LEU:HD12	2.26	0.51
1:A:132:LEU:HB3	1:A:134:LEU:HD13	1.90	0.51
1:B:127:ILE:HG21	1:B:130:SER:HA	1.92	0.51
1:E:364:GLU:CD	1:E:364:GLU:H	2.18	0.51
1:F:21:TYR:O	1:F:25:VAL:HG12	2.11	0.51
1:C:237:ASN:HD21	1:C:248:GLU:HB3	1.74	0.51
1:C:346:GLU:CD	1:C:346:GLU:H	2.18	0.51
1:D:237:ASN:ND2	1:D:248:GLU:HB3	2.25	0.51
1:F:305:HIS:HB3	1:F:445:TYR:OH	2.11	0.51
1:B:275:LEU:C	1:B:275:LEU:HD23	2.36	0.51
1:D:367:LYS:HB3	1:E:71:THR:HG21	1.93	0.51
1:F:291:HIS:O	1:F:294:VAL:HG22	2.11	0.51
1:B:381:ARG:O	1:B:381:ARG:HG3	2.11	0.51
1:D:36:ILE:HG23	1:D:138:MSE:CE	2.40	0.51
1:F:310:ARG:HB2	1:F:313:GLN:HG3	1.92	0.51
1:A:9:THR:HG23	1:A:12:GLN:HE21	1.76	0.51
1:B:310:ARG:H	1:B:313:GLN:HE21	1.59	0.51
1:D:306:CYS:HB3	1:D:424:LEU:HD13	1.93	0.51
1:A:14:LEU:HD13	1:A:94:ARG:HD3	1.92	0.50
1:E:151:LEU:CD2	1:F:431:LEU:HD12	2.41	0.50
1:F:127:ILE:HD13	1:F:132:LEU:CG	2.38	0.50
1:C:335:LEU:HD21	1:C:341:ILE:HD11	1.91	0.50
1:E:357:LEU:HD13	1:E:458:ARG:NH1	2.26	0.50
1:D:132:LEU:CB	1:D:134:LEU:HD11	2.41	0.50
1:D:436:LYS:NZ	1:D:436:LYS:HB3	2.26	0.50
1:E:29:ARG:HH21	1:E:128:ASP:HB2	1.76	0.50
1:E:261:PRO:HB2	1:E:263:TRP:CZ3	2.47	0.50
1:F:430:PRO:HA	1:F:435:ILE:HG12	1.92	0.50
1:A:36:ILE:HG23	1:A:138:MSE:CE	2.41	0.50
1:A:296:ARG:HD3	1:A:484:ARG:OXT	2.11	0.50
1:A:187:ARG:HG3	1:A:187:ARG:NH1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LEU:HB3	1:C:112:ILE:O	2.12	0.50
1:C:32:ILE:O	1:C:36:ILE:HG13	2.11	0.50
1:E:329:HIS:HD2	1:E:379:ASP:OD2	1.94	0.50
1:F:127:ILE:O	1:F:127:ILE:HG22	2.10	0.50
1:A:311:GLU:HB3	1:A:432:HIS:NE2	2.27	0.50
1:D:395:ASN:HD22	1:E:478:PHE:HD1	1.60	0.50
1:F:187:ARG:HG3	1:F:187:ARG:NH1	2.26	0.50
1:B:132:LEU:O	1:B:134:LEU:CD1	2.60	0.50
1:E:9:THR:HG22	1:E:105:TYR:OH	2.12	0.50
1:A:51:LEU:HD13	1:A:52:PHE:CE2	2.46	0.50
1:E:36:ILE:HG23	1:E:138:MSE:CE	2.41	0.50
1:A:463:LEU:HD22	1:A:470:LEU:HD13	1.93	0.49
1:A:291:HIS:O	1:A:294:VAL:HG22	2.12	0.49
1:C:437:LEU:HD13	1:C:437:LEU:N	2.26	0.49
1:D:430:PRO:HA	1:D:435:ILE:HG12	1.94	0.49
1:E:393:ARG:HH11	1:E:393:ARG:HG2	1.77	0.49
1:A:381:ARG:O	1:A:381:ARG:HG3	2.10	0.49
1:B:54:TYR:CD2	1:B:176:ALA:HB1	2.47	0.49
1:B:326:ARG:HG2	1:B:326:ARG:NH1	2.21	0.49
1:C:427:SER:O	1:C:428:ASP:HB3	2.12	0.49
1:E:31:ALA:HB1	1:E:42:PRO:HG3	1.95	0.49
1:A:352:TYR:CE2	1:A:356:LYS:HE3	2.47	0.49
1:D:31:ALA:HB1	1:D:42:PRO:HG3	1.93	0.49
1:E:357:LEU:HD13	1:E:458:ARG:HH11	1.77	0.49
1:B:28:LEU:O	1:B:32:ILE:HG13	2.12	0.49
1:B:228:TYR:CD1	1:B:265:LEU:HD13	2.48	0.49
1:B:322:HIS:CD2	1:C:474:LYS:HD3	2.48	0.49
1:C:463:LEU:HD22	1:C:470:LEU:HD13	1.95	0.49
1:E:63:GLY:CA	1:E:80:ALA:HB2	2.43	0.49
1:B:123:TYR:O	1:B:126:VAL:HG22	2.13	0.49
1:C:21:TYR:O	1:C:25:VAL:HG12	2.12	0.49
1:E:151:LEU:HG	1:F:384:GLU:HB3	1.95	0.49
1:E:417:ARG:HA	1:E:475:LEU:HD13	1.93	0.49
1:A:173:HIS:HE1	1:A:480:GLU:OE2	1.95	0.49
1:A:21:TYR:O	1:A:25:VAL:HG12	2.12	0.48
1:C:134:LEU:HD23	1:C:138:MSE:HE3	1.96	0.48
1:D:310:ARG:H	1:D:313:GLN:HE21	1.59	0.48
1:A:431:LEU:HD12	1:B:151:LEU:HD23	1.95	0.48
1:C:296:ARG:HD3	1:C:484:ARG:OXT	2.13	0.48
1:E:310:ARG:O	1:E:429:LYS:NZ	2.45	0.48
1:B:356:LYS:HE2	1:B:363:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LEU:HD13	1:B:458:ARG:NH1	2.27	0.48
1:C:173:HIS:HE1	1:C:480:GLU:OE2	1.95	0.48
1:A:228:TYR:CG	1:A:265:LEU:HD13	2.48	0.48
1:B:362:PRO:HD2	2:B:493:HOH:O	2.12	0.48
1:C:381:ARG:O	1:C:381:ARG:HG3	2.11	0.48
1:F:31:ALA:HB1	1:F:42:PRO:HG3	1.96	0.48
1:A:206:TYR:HB3	1:A:209:TYR:CD2	2.48	0.48
1:C:364:GLU:CD	1:C:364:GLU:H	2.22	0.48
1:C:440:GLN:HG2	1:C:441:ALA:H	1.79	0.48
1:D:291:HIS:O	1:D:294:VAL:HG22	2.13	0.48
1:F:357:LEU:HD13	1:F:458:ARG:HH11	1.78	0.48
1:A:8:LEU:HB3	1:A:112:ILE:O	2.13	0.48
1:B:477:THR:HB	1:C:395:ASN:HD21	1.79	0.48
1:D:173:HIS:HE1	1:D:480:GLU:OE2	1.97	0.48
1:E:32:ILE:O	1:E:36:ILE:HG13	2.14	0.48
1:B:474:LYS:HD3	1:C:322:HIS:HD2	1.79	0.48
1:C:291:HIS:O	1:C:294:VAL:HG22	2.14	0.48
1:F:275:LEU:C	1:F:275:LEU:HD23	2.38	0.48
1:D:311:GLU:HB3	1:D:432:HIS:NE2	2.29	0.48
1:F:9:THR:HG23	1:F:12:GLN:NE2	2.28	0.48
1:B:216:TRP:O	1:B:220:GLN:HG2	2.14	0.47
1:F:89:ARG:N	1:F:90:PRO:HD3	2.29	0.47
1:A:305:HIS:HB2	1:A:427:SER:HB3	1.96	0.47
1:A:346:GLU:H	1:A:346:GLU:CD	2.22	0.47
1:B:463:LEU:HD22	1:B:470:LEU:HD13	1.95	0.47
1:C:123:TYR:O	1:C:126:VAL:HG22	2.14	0.47
1:D:9:THR:HG22	1:D:105:TYR:OH	2.14	0.47
1:D:134:LEU:N	1:D:134:LEU:HD12	2.30	0.47
1:A:53:VAL:HG11	1:A:117:SER:O	2.15	0.47
1:A:260:MSE:HG2	1:A:278:ILE:HA	1.96	0.47
1:B:190:THR:HG22	1:B:192:THR:CB	2.33	0.47
1:C:63:GLY:CA	1:C:80:ALA:HB2	2.44	0.47
1:E:260:MSE:HG2	1:E:278:ILE:HA	1.95	0.47
1:E:393:ARG:HG2	1:E:393:ARG:NH1	2.29	0.47
1:E:427:SER:O	1:E:428:ASP:HB3	2.15	0.47
1:F:335:LEU:HD21	1:F:341:ILE:HD11	1.96	0.47
1:E:28:LEU:HD13	1:E:126:VAL:HG21	1.96	0.47
1:C:134:LEU:HD12	1:C:134:LEU:N	2.30	0.47
1:F:190:THR:HG23	1:F:262:ALA:CB	2.39	0.47
1:C:55:PRO:HD2	1:C:87:ILE:O	2.14	0.47
1:C:136:ARG:HG3	1:D:444:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:ARG:HA	1:D:475:LEU:HD13	1.96	0.47
1:F:175:ASP:O	1:F:179:VAL:HG23	2.13	0.47
1:A:369:ARG:HG2	1:A:369:ARG:HH11	1.80	0.47
1:C:136:ARG:NH2	1:D:444:PHE:HB3	2.29	0.47
1:C:206:TYR:HB3	1:C:209:TYR:CD2	2.50	0.47
1:D:352:TYR:CE2	1:D:356:LYS:HE3	2.48	0.47
1:B:54:TYR:CE2	1:B:176:ALA:HB1	2.50	0.47
1:B:355:THR:O	1:B:359:SER:HB3	2.14	0.47
1:C:9:THR:HG23	1:C:12:GLN:NE2	2.28	0.47
1:A:431:LEU:HD12	1:B:151:LEU:CD2	2.45	0.47
1:B:305:HIS:HB2	1:B:427:SER:HB3	1.97	0.47
1:C:9:THR:HG22	1:C:105:TYR:OH	2.15	0.47
1:C:123:TYR:CG	1:C:124:PRO:HD3	2.50	0.47
1:E:356:LYS:HE2	1:E:363:GLY:H	1.79	0.47
1:F:346:GLU:H	1:F:346:GLU:CD	2.22	0.47
1:B:127:ILE:HG22	1:B:127:ILE:O	2.14	0.46
1:B:430:PRO:HA	1:B:435:ILE:HG12	1.97	0.46
1:D:296:ARG:HD3	1:D:484:ARG:OXT	2.15	0.46
1:E:9:THR:HG23	1:E:12:GLN:NE2	2.29	0.46
1:E:361:ARG:N	1:E:362:PRO:HD3	2.30	0.46
1:F:206:TYR:HB3	1:F:209:TYR:CD2	2.51	0.46
1:A:29:ARG:NH2	1:A:128:ASP:HB2	2.31	0.46
1:A:134:LEU:N	1:A:134:LEU:HD12	2.30	0.46
1:A:357:LEU:HD13	1:A:458:ARG:NH1	2.31	0.46
1:B:151:LEU:O	1:B:153:GLN:HG2	2.15	0.46
1:B:261:PRO:HB2	1:B:263:TRP:CZ3	2.50	0.46
1:F:190:THR:HG22	1:F:192:THR:CB	2.30	0.46
1:A:123:TYR:CG	1:A:124:PRO:HD3	2.50	0.46
1:F:463:LEU:HD22	1:F:470:LEU:HD13	1.97	0.46
1:A:190:THR:HG22	1:A:192:THR:N	2.30	0.46
1:C:361:ARG:HB3	1:C:365:GLU:HB2	1.97	0.46
1:C:396:LEU:HD12	1:C:396:LEU:HA	1.78	0.46
1:E:259:GLN:OE1	1:F:280:VAL:HG11	2.16	0.46
1:F:8:LEU:HB3	1:F:112:ILE:O	2.16	0.46
1:C:136:ARG:HH22	1:D:444:PHE:HB3	1.80	0.46
1:D:361:ARG:HG3	1:D:361:ARG:HH11	1.81	0.46
1:A:9:THR:HG22	1:A:105:TYR:OH	2.16	0.46
1:A:61:TRP:CE2	1:A:108:TYR:HD2	2.34	0.46
1:C:435:ILE:C	1:C:436:LYS:HG3	2.40	0.46
1:E:77:PHE:CE2	1:E:104:LEU:HD22	2.50	0.46
1:A:31:ALA:HB1	1:A:42:PRO:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ARG:O	1:F:398:ARG:HD2	2.15	0.46
1:D:91:THR:HB	2:D:493:HOH:O	2.16	0.46
1:E:215:ARG:NH1	1:E:215:ARG:HG2	2.29	0.46
1:A:206:TYR:HB3	1:A:209:TYR:HD2	1.80	0.46
1:D:206:TYR:HB3	1:D:209:TYR:CD2	2.51	0.46
1:D:36:ILE:HA	1:D:138:MSE:HE1	1.97	0.46
1:F:357:LEU:HD13	1:F:458:ARG:NH1	2.30	0.46
1:B:31:ALA:HB1	1:B:42:PRO:HG3	1.98	0.46
1:F:134:LEU:HB3	1:F:138:MSE:CB	2.46	0.46
1:A:336:PRO:HA	1:A:337:PRO:HD3	1.81	0.45
1:B:260:MSE:HG2	1:B:278:ILE:HA	1.98	0.45
1:B:357:LEU:HD13	1:B:458:ARG:HH11	1.81	0.45
1:C:89:ARG:N	1:C:90:PRO:HD3	2.31	0.45
1:B:105:TYR:O	1:B:109:GLY:HA2	2.17	0.45
1:C:142:LEU:HD23	1:C:146:PHE:CD2	2.52	0.45
1:C:444:PHE:CZ	1:D:136:ARG:HG3	2.51	0.45
1:E:310:ARG:HB2	1:E:313:GLN:HG3	1.98	0.45
1:E:105:TYR:O	1:E:109:GLY:HA2	2.15	0.45
1:E:190:THR:HG22	1:E:192:THR:CB	2.34	0.45
1:F:9:THR:HG22	1:F:105:TYR:OH	2.16	0.45
1:F:427:SER:O	1:F:428:ASP:HB3	2.15	0.45
1:C:357:LEU:HD13	1:C:458:ARG:NH1	2.32	0.45
1:C:14:LEU:HD13	1:C:94:ARG:HD3	1.98	0.45
1:C:31:ALA:HB1	1:C:42:PRO:HG3	1.98	0.45
1:C:206:TYR:HB3	1:C:209:TYR:HD2	1.81	0.45
1:C:357:LEU:HD13	1:C:458:ARG:HH11	1.81	0.45
1:D:71:THR:HG23	1:E:367:LYS:HB3	1.99	0.45
1:B:222:LEU:O	1:B:224:PRO:HD3	2.17	0.45
1:C:390:SER:HB3	1:C:394:PHE:CE1	2.52	0.45
1:B:63:GLY:CA	1:B:80:ALA:HB2	2.47	0.45
1:C:305:HIS:HB2	1:C:427:SER:HB3	1.98	0.45
1:E:237:ASN:ND2	1:E:248:GLU:HB3	2.32	0.45
1:A:443:ARG:HE	1:B:133:THR:HB	1.81	0.45
1:F:105:TYR:O	1:F:109:GLY:HA2	2.17	0.45
1:A:261:PRO:HB2	1:A:263:TRP:CZ3	2.52	0.45
1:B:417:ARG:HA	1:B:475:LEU:HD13	1.99	0.45
1:E:215:ARG:HG2	1:E:215:ARG:HH11	1.81	0.45
1:B:398:ARG:HD3	1:C:477:THR:HG22	1.98	0.44
1:D:123:TYR:O	1:D:126:VAL:HG22	2.17	0.44
1:D:134:LEU:HB3	1:D:138:MSE:HB2	1.98	0.44
1:D:265:LEU:HD23	1:D:265:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:GLU:CD	1:E:346:GLU:H	2.25	0.44
1:F:237:ASN:HD21	1:F:248:GLU:CB	2.30	0.44
1:F:306:CYS:HB3	1:F:424:LEU:HD13	1.99	0.44
1:E:450:SER:HB3	2:E:507:HOH:O	2.17	0.44
1:A:134:LEU:HB3	1:A:138:MSE:HB2	1.99	0.44
1:A:364:GLU:O	1:A:364:GLU:HG2	2.17	0.44
1:E:53:VAL:HG11	1:E:117:SER:O	2.18	0.44
1:F:206:TYR:HB3	1:F:209:TYR:HD2	1.82	0.44
1:A:360:GLY:C	1:A:362:PRO:HD3	2.42	0.44
1:C:364:GLU:CD	1:C:364:GLU:N	2.76	0.44
1:E:296:ARG:HD3	1:E:484:ARG:OXT	2.18	0.44
1:E:306:CYS:HB3	1:E:424:LEU:HD13	1.99	0.44
1:F:417:ARG:HA	1:F:475:LEU:HD13	1.99	0.44
1:B:127:ILE:HG22	1:B:130:SER:HA	1.99	0.44
1:B:428:ASP:HB3	1:B:436:LYS:HB2	2.00	0.44
1:D:105:TYR:O	1:D:109:GLY:HA2	2.17	0.44
1:F:381:ARG:O	1:F:381:ARG:HG3	2.18	0.44
1:A:361:ARG:O	1:A:366:VAL:HG13	2.17	0.44
1:A:440:GLN:NE2	1:A:441:ALA:H	2.16	0.44
1:D:261:PRO:HB2	1:D:263:TRP:CZ3	2.53	0.44
1:F:237:ASN:ND2	1:F:248:GLU:HB3	2.32	0.44
1:F:261:PRO:HB2	1:F:263:TRP:CZ3	2.52	0.44
1:F:363:GLY:O	1:F:364:GLU:HB3	2.18	0.44
1:A:134:LEU:CD2	1:A:138:MSE:HE3	2.48	0.44
1:B:9:THR:HG23	1:B:12:GLN:NE2	2.32	0.44
1:D:365:GLU:OE1	1:D:365:GLU:HA	2.18	0.44
1:A:63:GLY:CA	1:A:80:ALA:HB2	2.48	0.44
1:C:105:TYR:O	1:C:109:GLY:HA2	2.17	0.44
1:C:252:ASP:OD1	1:D:253:LEU:HD13	2.17	0.44
1:D:9:THR:HG23	1:D:12:GLN:NE2	2.31	0.44
1:F:134:LEU:HD23	1:F:138:MSE:HE3	2.00	0.44
1:A:190:THR:HG22	1:A:192:THR:CB	2.34	0.44
1:B:122:PRO:HA	1:B:147:PRO:O	2.18	0.44
1:C:61:TRP:CE2	1:C:108:TYR:HD2	2.35	0.44
1:C:228:TYR:HB3	1:C:265:LEU:HD22	1.98	0.44
1:C:261:PRO:HB2	1:C:263:TRP:CZ3	2.53	0.44
1:C:437:LEU:HD21	1:C:440:GLN:CD	2.43	0.44
1:D:134:LEU:HB3	1:D:138:MSE:CB	2.48	0.44
1:E:55:PRO:HD2	1:E:87:ILE:O	2.18	0.44
1:A:296:ARG:N	1:A:297:PRO:HD3	2.33	0.43
1:B:264:HIS:CE1	1:B:274:THR:HG23	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:LYS:HD3	1:E:322:HIS:HD2	1.83	0.43
1:A:216:TRP:O	1:A:220:GLN:HG2	2.18	0.43
1:A:237:ASN:ND2	1:A:248:GLU:HB3	2.33	0.43
1:E:134:LEU:HD23	1:E:138:MSE:HE3	1.99	0.43
1:E:443:ARG:HB2	1:F:133:THR:CG2	2.48	0.43
1:B:123:TYR:CG	1:B:124:PRO:HD3	2.54	0.43
1:D:216:TRP:O	1:D:220:GLN:HG2	2.19	0.43
1:A:54:TYR:CD2	1:A:176:ALA:HB1	2.54	0.43
1:A:395:ASN:HD22	1:F:478:PHE:HD1	1.67	0.43
1:A:440:GLN:HA	1:A:440:GLN:NE2	2.33	0.43
1:A:478:PHE:HD1	1:F:395:ASN:HD22	1.66	0.43
1:C:437:LEU:HD21	1:C:440:GLN:OE1	2.18	0.43
1:D:127:ILE:O	1:D:127:ILE:HG22	2.17	0.43
1:D:296:ARG:N	1:D:297:PRO:HD3	2.33	0.43
1:F:9:THR:HB	1:F:10:PRO:HD2	1.99	0.43
1:C:296:ARG:N	1:C:297:PRO:HD3	2.32	0.43
1:D:309:LEU:N	1:D:313:GLN:HE22	2.17	0.43
1:E:36:ILE:HA	1:E:138:MSE:HE1	1.99	0.43
1:F:247:GLU:C	1:F:249:ALA:H	2.26	0.43
1:A:395:ASN:HD22	1:A:395:ASN:HA	1.69	0.43
1:B:127:ILE:HG22	1:B:130:SER:CA	2.48	0.43
1:C:77:PHE:CE2	1:C:104:LEU:HD22	2.54	0.43
1:C:215:ARG:NH1	1:C:215:ARG:HG2	2.34	0.43
1:C:418:VAL:O	1:C:419:PRO:C	2.61	0.43
1:D:333:ALA:HB3	2:D:523:HOH:O	2.18	0.43
1:A:266:ILE:HG22	1:A:267:THR:N	2.32	0.43
1:D:357:LEU:HD13	1:D:458:ARG:NH1	2.33	0.43
1:D:437:LEU:HB2	1:D:440:GLN:CD	2.43	0.43
1:E:132:LEU:HB3	1:E:134:LEU:HD13	2.00	0.43
1:F:128:ASP:O	1:F:129:GLY:O	2.37	0.43
1:F:215:ARG:NH1	1:F:215:ARG:HG2	2.34	0.43
1:A:351:LEU:HG	1:A:423:LEU:HB2	2.01	0.43
1:B:53:VAL:HG11	1:B:117:SER:O	2.19	0.43
1:E:336:PRO:HA	1:E:337:PRO:HD3	1.82	0.43
1:B:54:TYR:CE1	1:B:121:ILE:HA	2.54	0.43
1:C:244:GLU:C	1:C:246:PRO:HD3	2.44	0.43
1:D:123:TYR:CG	1:D:124:PRO:HD3	2.54	0.43
1:E:134:LEU:CD2	1:E:138:MSE:HE3	2.49	0.43
1:E:136:ARG:NH2	1:F:444:PHE:HB3	2.34	0.43
1:E:361:ARG:HB3	1:E:365:GLU:CB	2.38	0.43
1:B:212:GLU:HG2	1:B:450:SER:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:THR:HB	1:C:10:PRO:HD2	2.01	0.42
1:D:63:GLY:CA	1:D:80:ALA:HB2	2.48	0.42
1:D:132:LEU:C	1:D:134:LEU:HD12	2.44	0.42
1:E:237:ASN:HD21	1:E:248:GLU:CB	2.31	0.42
1:A:437:LEU:HD12	1:A:437:LEU:N	2.34	0.42
1:B:68:PRO:HA	1:B:69:PRO:HD3	1.97	0.42
1:D:206:TYR:HB3	1:D:209:TYR:HD2	1.84	0.42
1:D:344:ILE:O	1:D:348:GLN:HG2	2.19	0.42
1:F:216:TRP:O	1:F:220:GLN:HG2	2.19	0.42
1:F:288:ILE:HD12	1:F:288:ILE:HA	1.88	0.42
1:A:247:GLU:C	1:A:249:ALA:H	2.27	0.42
1:B:280:VAL:HA	1:B:405:GLU:OE2	2.20	0.42
1:C:16:LYS:HD3	1:C:114:VAL:HB	2.01	0.42
1:C:395:ASN:HD22	1:C:395:ASN:HA	1.68	0.42
1:E:259:GLN:HE22	1:F:381:ARG:HH12	1.67	0.42
1:F:266:ILE:HG22	1:F:267:THR:N	2.33	0.42
1:A:134:LEU:HB3	1:A:138:MSE:CB	2.49	0.42
1:A:357:LEU:HD13	1:A:458:ARG:HH11	1.85	0.42
1:B:266:ILE:HG22	1:B:267:THR:N	2.33	0.42
1:A:310:ARG:HB2	1:A:313:GLN:HG3	2.01	0.42
1:C:120:GLU:OE1	1:C:147:PRO:HG3	2.18	0.42
1:C:132:LEU:HB3	1:C:134:LEU:CD1	2.48	0.42
1:C:260:MSE:HG2	1:C:278:ILE:HA	2.02	0.42
1:C:265:LEU:HD23	1:C:265:LEU:HA	1.71	0.42
1:D:8:LEU:HB3	1:D:112:ILE:O	2.20	0.42
1:D:280:VAL:HA	1:D:405:GLU:OE2	2.18	0.42
1:D:275:LEU:C	1:D:275:LEU:HD23	2.45	0.42
1:E:134:LEU:HD12	1:E:134:LEU:H	1.84	0.42
1:E:206:TYR:HB3	1:E:209:TYR:CD2	2.55	0.42
1:E:309:LEU:N	1:E:313:GLN:HE22	2.17	0.42
1:E:151:LEU:HD11	1:F:435:ILE:HD11	2.01	0.42
1:F:29:ARG:HH21	1:F:128:ASP:HB2	1.83	0.42
1:C:134:LEU:CD2	1:C:138:MSE:HE3	2.50	0.42
1:C:310:ARG:HB2	1:C:313:GLN:HG3	2.01	0.42
1:D:396:LEU:HD12	1:D:396:LEU:HA	1.90	0.42
1:E:296:ARG:N	1:E:297:PRO:HD3	2.35	0.42
1:F:134:LEU:CD1	1:F:134:LEU:N	2.83	0.42
1:A:216:TRP:HZ3	1:A:265:LEU:HD12	1.84	0.42
1:C:96:TYR:OH	1:C:483:PHE:HB3	2.20	0.42
1:D:244:GLU:C	1:D:246:PRO:HD3	2.43	0.42
1:D:346:GLU:CD	1:D:346:GLU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:LEU:HA	1:E:265:LEU:HD23	1.75	0.42
1:F:351:LEU:HG	1:F:423:LEU:HB2	2.02	0.42
1:B:16:LYS:HD3	1:B:114:VAL:HB	2.01	0.42
1:B:32:ILE:O	1:B:36:ILE:HG13	2.19	0.42
1:C:47:ARG:HA	1:C:51:LEU:HB2	2.02	0.42
1:C:188:HIS:CE1	1:D:438:PRO:O	2.73	0.42
1:D:260:MSE:HG2	1:D:278:ILE:HA	2.02	0.42
1:E:247:GLU:C	1:E:249:ALA:H	2.26	0.42
1:A:55:PRO:HD2	1:A:87:ILE:O	2.20	0.41
1:B:9:THR:HG22	1:B:105:TYR:OH	2.19	0.41
1:B:296:ARG:N	1:B:297:PRO:HD3	2.34	0.41
1:B:359:SER:HA	1:B:451:GLU:OE1	2.20	0.41
1:C:122:PRO:HA	1:C:147:PRO:O	2.19	0.41
1:F:286:LYS:HD2	1:F:330:VAL:HG22	2.01	0.41
1:F:480:GLU:HA	1:F:481:PRO:HD3	1.95	0.41
1:B:351:LEU:HD12	1:B:351:LEU:HA	1.94	0.41
1:C:190:THR:HG21	1:C:192:THR:HB	1.94	0.41
1:D:305:HIS:HB3	1:D:445:TYR:OH	2.19	0.41
1:D:481:PRO:HA	1:D:482:PRO:HD3	1.92	0.41
1:E:175:ASP:OD1	1:E:175:ASP:C	2.63	0.41
1:F:387:TYR:O	1:F:388:SER:C	2.64	0.41
1:A:326:ARG:NH1	1:A:326:ARG:CG	2.77	0.41
1:C:247:GLU:C	1:C:249:ALA:H	2.28	0.41
1:E:395:ASN:HD22	1:E:395:ASN:HA	1.72	0.41
1:F:51:LEU:HD13	1:F:52:PHE:CE2	2.55	0.41
1:F:56:SER:HB3	1:F:115:GLN:O	2.20	0.41
1:F:123:TYR:O	1:F:126:VAL:HG22	2.20	0.41
1:A:123:TYR:O	1:A:126:VAL:HG22	2.21	0.41
1:D:237:ASN:HD21	1:D:248:GLU:CB	2.30	0.41
1:D:356:LYS:O	1:D:360:GLY:N	2.50	0.41
1:D:398:ARG:HD3	1:E:477:THR:HG22	2.01	0.41
1:E:178:ARG:NH2	1:E:290:ASP:O	2.53	0.41
1:F:134:LEU:HB3	1:F:138:MSE:HB2	2.03	0.41
1:C:435:ILE:O	1:C:436:LYS:HG3	2.21	0.41
1:E:134:LEU:HB3	1:E:138:MSE:CB	2.51	0.41
1:E:309:LEU:H	1:E:313:GLN:HE22	1.69	0.41
1:F:63:GLY:CA	1:F:80:ALA:HB2	2.50	0.41
1:A:259:GLN:OE1	1:B:280:VAL:HG11	2.20	0.41
1:A:440:GLN:CD	1:A:441:ALA:N	2.78	0.41
1:B:151:LEU:C	1:B:153:GLN:N	2.78	0.41
1:B:228:TYR:HB3	1:B:265:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:THR:HB	1:D:10:PRO:HD2	2.03	0.41
1:F:280:VAL:HA	1:F:405:GLU:OE2	2.20	0.41
1:F:310:ARG:N	1:F:313:GLN:HE21	2.01	0.41
1:A:105:TYR:O	1:A:109:GLY:HA2	2.20	0.41
1:B:29:ARG:NH2	1:B:128:ASP:HB2	2.36	0.41
1:C:134:LEU:N	1:C:134:LEU:CD1	2.83	0.41
1:C:351:LEU:HG	1:C:423:LEU:HB2	2.03	0.41
1:D:347:VAL:HG12	1:D:351:LEU:HD22	2.03	0.41
1:A:68:PRO:HA	1:A:69:PRO:HD3	1.99	0.41
1:A:275:LEU:C	1:A:275:LEU:HD23	2.45	0.41
1:D:123:TYR:CD1	1:D:123:TYR:C	2.99	0.41
1:D:369:ARG:HH11	1:D:369:ARG:HG2	1.85	0.41
1:D:480:GLU:HA	1:D:481:PRO:HD3	1.96	0.41
1:E:16:LYS:HD3	1:E:114:VAL:HB	2.02	0.41
1:E:56:SER:HB3	1:E:115:GLN:O	2.20	0.41
1:E:192:THR:HA	1:E:193:PRO:HD3	1.90	0.41
1:F:355:THR:O	1:F:359:SER:HB3	2.21	0.41
1:A:201:VAL:HG12	1:A:202:LEU:N	2.36	0.41
1:A:211:ASP:HA	1:A:250:ILE:CD1	2.51	0.41
1:A:305:HIS:HB3	1:A:445:TYR:OH	2.21	0.41
1:A:322:HIS:HD2	1:F:474:LYS:HD3	1.86	0.41
1:A:440:GLN:CD	1:A:441:ALA:H	2.29	0.41
1:A:474:LYS:HD3	1:F:322:HIS:HD2	1.86	0.41
1:B:72:ARG:HG2	1:B:74:PHE:O	2.21	0.41
1:B:309:LEU:N	1:B:313:GLN:HE22	2.19	0.41
1:B:423:LEU:HD22	1:B:455:ILE:HG21	2.02	0.41
1:C:215:ARG:HG2	1:C:215:ARG:HH11	1.86	0.41
1:C:228:TYR:CG	1:C:265:LEU:HD13	2.55	0.41
1:C:259:GLN:C	1:C:260:MSE:HG3	2.46	0.41
1:D:336:PRO:HA	1:D:337:PRO:HD3	1.83	0.41
1:D:427:SER:O	1:D:428:ASP:HB3	2.21	0.41
1:D:478:PHE:HD1	1:E:395:ASN:HD22	1.68	0.41
1:E:226:SER:HA	1:E:227:PRO:HD3	1.85	0.41
1:F:173:HIS:HE1	1:F:480:GLU:OE2	2.04	0.41
1:F:296:ARG:N	1:F:297:PRO:HD3	2.35	0.41
1:A:190:THR:HG23	1:A:192:THR:HB	1.90	0.41
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.87	0.41
1:C:305:HIS:HB3	1:C:445:TYR:OH	2.21	0.41
1:D:61:TRP:CE3	1:D:63:GLY:HA2	2.56	0.41
1:D:61:TRP:CE2	1:D:108:TYR:HD2	2.39	0.41
1:D:418:VAL:O	1:D:419:PRO:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:PHE:HD2	1:F:136:ARG:NH2	2.19	0.41
1:F:16:LYS:HD3	1:F:114:VAL:HB	2.03	0.41
1:F:264:HIS:CE1	1:F:274:THR:HG23	2.56	0.41
1:A:228:TYR:HB3	1:A:265:LEU:HD22	2.01	0.40
1:B:206:TYR:HB3	1:B:209:TYR:CD2	2.56	0.40
1:A:245:ALA:C	1:A:247:GLU:H	2.29	0.40
1:B:245:ALA:C	1:B:247:GLU:H	2.29	0.40
1:B:427:SER:O	1:B:428:ASP:HB3	2.21	0.40
1:C:169:SER:HA	1:C:170:PRO:HD3	1.79	0.40
1:C:481:PRO:HA	1:C:482:PRO:HD3	1.92	0.40
1:D:89:ARG:N	1:D:90:PRO:HD3	2.36	0.40
1:F:168:PHE:O	1:F:168:PHE:HD1	2.04	0.40
1:A:223:ASP:OD2	1:A:223:ASP:C	2.62	0.40
1:B:134:LEU:HD12	1:B:134:LEU:N	2.36	0.40
1:B:175:ASP:O	1:B:179:VAL:HG23	2.21	0.40
1:B:215:ARG:NH1	1:B:215:ARG:HG2	2.36	0.40
1:B:395:ASN:HD21	1:C:478:PHE:H	1.68	0.40
1:D:245:ALA:C	1:D:247:GLU:H	2.29	0.40
1:E:423:LEU:HD22	1:E:455:ILE:HG21	2.02	0.40
1:A:192:THR:HA	1:A:193:PRO:HD3	1.90	0.40
1:B:89:ARG:N	1:B:90:PRO:HD3	2.37	0.40
1:B:395:ASN:HD22	1:B:395:ASN:HA	1.72	0.40
1:E:444:PHE:CD2	1:F:136:ARG:NH2	2.89	0.40
1:F:212:GLU:HG2	1:F:450:SER:HA	2.04	0.40
1:A:344:ILE:O	1:A:348:GLN:HG2	2.22	0.40
1:B:281:GLY:HA2	1:B:282:PRO:HD3	1.97	0.40
1:B:310:ARG:HB2	1:B:313:GLN:HG3	2.03	0.40
1:B:336:PRO:HA	1:B:337:PRO:HD3	1.85	0.40
1:B:442:ASN:O	1:B:443:ARG:C	2.65	0.40
1:B:478:PHE:CD1	1:C:395:ASN:ND2	2.86	0.40
1:C:53:VAL:HG11	1:C:117:SER:O	2.21	0.40
1:C:226:SER:HA	1:C:227:PRO:HD3	1.85	0.40
1:E:266:ILE:HG22	1:E:267:THR:N	2.36	0.40
1:E:435:ILE:HD11	1:F:151:LEU:CD1	2.44	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	459/484 (95%)	426 (93%)	28 (6%)	5 (1%)	11	29
1	B	459/484 (95%)	428 (93%)	28 (6%)	3 (1%)	18	41
1	C	459/484 (95%)	426 (93%)	30 (6%)	3 (1%)	18	41
1	D	459/484 (95%)	432 (94%)	23 (5%)	4 (1%)	14	35
1	E	459/484 (95%)	434 (95%)	21 (5%)	4 (1%)	14	35
1	F	459/484 (95%)	424 (92%)	30 (6%)	5 (1%)	11	29
All	All	2754/2904 (95%)	2570 (93%)	160 (6%)	24 (1%)	14	35

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	B	66	THR
1	C	66	THR
1	D	66	THR
1	E	66	THR
1	F	66	THR
1	F	362	PRO
1	A	129	GLY
1	C	129	GLY
1	D	130	SER
1	E	129	GLY
1	F	129	GLY
1	F	364	GLU
1	A	131	GLU
1	A	441	ALA
1	F	406	SER
1	B	406	SER
1	D	152	ALA
1	E	152	ALA
1	C	406	SER

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Mol	Chain	Res	Type
1	A	406	SER
1	B	152	ALA
1	D	406	SER
1	E	438	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/403 (97%)	367 (94%)	24 (6%)	17	40
1	B	391/403 (97%)	373 (95%)	18 (5%)	24	51
1	C	391/403 (97%)	369 (94%)	22 (6%)	19	44
1	D	391/403 (97%)	370 (95%)	21 (5%)	20	45
1	E	391/403 (97%)	372 (95%)	19 (5%)	22	49
1	F	391/403 (97%)	373 (95%)	18 (5%)	24	51
All	All	2346/2418 (97%)	2224 (95%)	122 (5%)	21	47

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	25	VAL
1	A	28	LEU
1	A	51	LEU
1	A	53	VAL
1	A	89	ARG
1	A	150	GLU
1	A	151	LEU
1	A	153	GLN
1	A	190	THR
1	A	202	LEU
1	A	210	VAL
1	A	222	LEU
1	A	248	GLU

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Mol	Chain	Res	Type
1	A	265	LEU
1	A	301	LEU
1	A	322	HIS
1	A	351	LEU
1	A	364	GLU
1	A	395	ASN
1	A	396	LEU
1	A	400	VAL
1	A	431	LEU
1	A	437	LEU
1	B	25	VAL
1	B	28	LEU
1	B	51	LEU
1	B	53	VAL
1	B	89	ARG
1	B	190	THR
1	B	202	LEU
1	B	210	VAL
1	B	222	LEU
1	B	248	GLU
1	B	265	LEU
1	B	301	LEU
1	B	322	HIS
1	B	351	LEU
1	B	364	GLU
1	B	396	LEU
1	B	400	VAL
1	B	431	LEU
1	C	18	ASP
1	C	25	VAL
1	C	28	LEU
1	C	51	LEU
1	C	53	VAL
1	C	89	ARG
1	C	133	THR
1	C	151	LEU
1	C	153	GLN
1	C	190	THR
1	C	202	LEU
1	C	210	VAL
1	C	222	LEU
1	C	248	GLU

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Mol	Chain	Res	Type
1	C	265	LEU
1	C	301	LEU
1	C	322	HIS
1	C	351	LEU
1	C	364	GLU
1	C	396	LEU
1	C	400	VAL
1	C	437	LEU
1	D	18	ASP
1	D	25	VAL
1	D	28	LEU
1	D	51	LEU
1	D	89	ARG
1	D	169	SER
1	D	190	THR
1	D	192	THR
1	D	202	LEU
1	D	210	VAL
1	D	222	LEU
1	D	248	GLU
1	D	265	LEU
1	D	301	LEU
1	D	322	HIS
1	D	351	LEU
1	D	396	LEU
1	D	400	VAL
1	D	431	LEU
1	D	436	LYS
1	D	443	ARG
1	E	18	ASP
1	E	25	VAL
1	E	28	LEU
1	E	51	LEU
1	E	53	VAL
1	E	133	THR
1	E	151	LEU
1	E	190	THR
1	E	202	LEU
1	E	210	VAL
1	E	222	LEU
1	E	248	GLU
1	E	265	LEU

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Mol	Chain	Res	Type
1	E	301	LEU
1	E	322	HIS
1	E	351	LEU
1	E	396	LEU
1	E	400	VAL
1	E	431	LEU
1	F	18	ASP
1	F	25	VAL
1	F	28	LEU
1	F	51	LEU
1	F	89	ARG
1	F	149	THR
1	F	190	THR
1	F	192	THR
1	F	202	LEU
1	F	210	VAL
1	F	222	LEU
1	F	248	GLU
1	F	265	LEU
1	F	301	LEU
1	F	322	HIS
1	F	351	LEU
1	F	400	VAL
1	F	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	173	HIS
1	A	237	ASN
1	A	284	ASN
1	A	313	GLN
1	A	322	HIS
1	A	329	HIS
1	A	348	GLN
1	A	395	ASN
1	A	440	GLN
1	B	12	GLN
1	B	173	HIS
1	B	237	ASN
1	B	284	ASN

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Mol	Chain	Res	Type
1	B	305	HIS
1	B	313	GLN
1	B	322	HIS
1	B	329	HIS
1	B	368	GLN
1	B	395	ASN
1	B	440	GLN
1	C	12	GLN
1	C	173	HIS
1	C	188	HIS
1	C	237	ASN
1	C	284	ASN
1	C	313	GLN
1	C	322	HIS
1	C	329	HIS
1	C	348	GLN
1	C	395	ASN
1	D	12	GLN
1	D	23	GLN
1	D	30	ASN
1	D	173	HIS
1	D	237	ASN
1	D	284	ASN
1	D	313	GLN
1	D	322	HIS
1	D	329	HIS
1	D	368	GLN
1	D	395	ASN
1	E	12	GLN
1	E	173	HIS
1	E	188	HIS
1	E	237	ASN
1	E	284	ASN
1	E	313	GLN
1	E	322	HIS
1	E	329	HIS
1	E	395	ASN
1	F	12	GLN
1	F	115	GLN
1	F	173	HIS
1	F	237	ASN
1	F	284	ASN

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Mol	Chain	Res	Type
1	F	313	GLN
1	F	322	HIS
1	F	329	HIS
1	F	348	GLN
1	F	395	ASN
1	F	442	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.