



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:17 PM UTC

PDB ID : 3BWO / pdb_00003bwo
Title : L-tryptophan aminotransferase
Authors : Ferrer, J.-L.; Noel, J.P.; Pojer, F.; Bowman, M.; Chory, J.; Tao, Y.
Deposited on : 2008-01-10
Resolution : 2.40 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

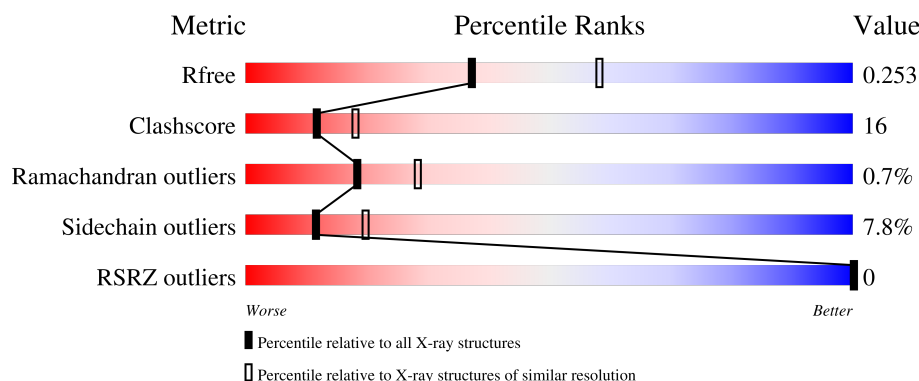
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	391	 66% 22% • • 7%
1	B	391	 63% 25% • • 7%
1	C	391	 63% 22% 6% • 8%
1	D	391	 60% 26% 5% • 8%
1	E	391	 65% 23% • 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	391	62% 24% 5% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18479 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-tryptophan aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	P	S	0	0	0
			2935	1863	499	553	1	19			
1	B	364	Total	C	N	O	P	S	0	0	0
			2943	1871	499	553	1	19			
1	C	360	Total	C	N	O	P	S	0	0	0
			2910	1849	493	548	1	19			
1	D	360	Total	C	N	O	P	S	0	0	0
			2909	1847	493	549	1	19			
1	E	361	Total	C	N	O	P	S	0	0	0
			2920	1856	495	549	1	19			
1	F	363	Total	C	N	O	P	S	0	0	0
			2935	1867	497	551	1	19			

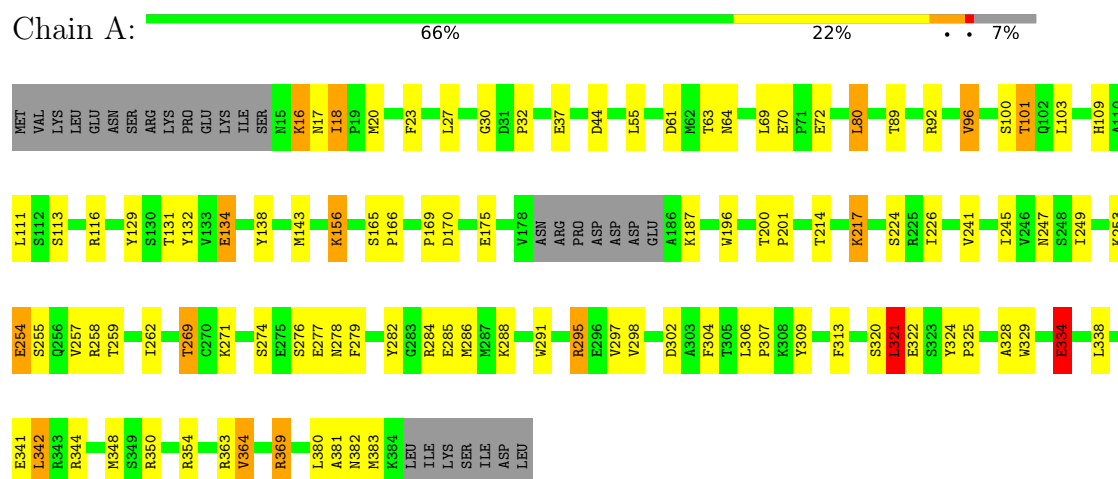
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	161	Total	O	0	0
			161	161		
2	B	184	Total	O	0	0
			184	184		
2	C	132	Total	O	0	0
			132	132		
2	D	159	Total	O	0	0
			159	159		
2	E	135	Total	O	0	0
			135	135		
2	F	156	Total	O	0	0
			156	156		

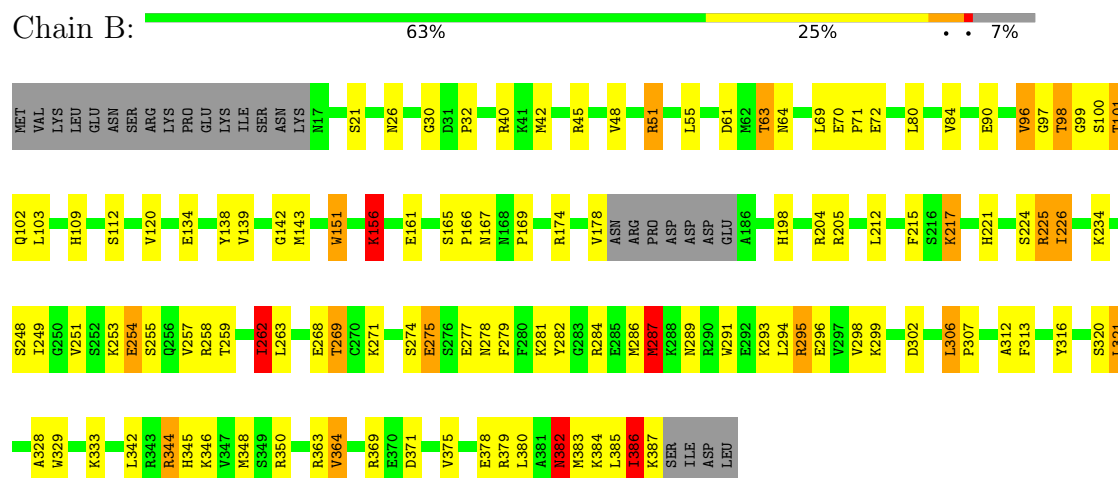
3 Residue-property plots

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 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-tryptophan aminotransferase

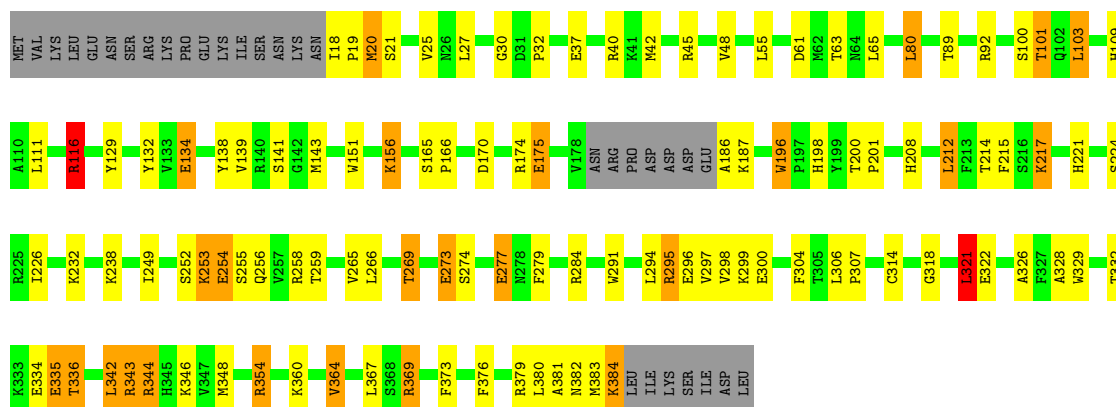


• Molecule 1: L-tryptophan aminotransferase



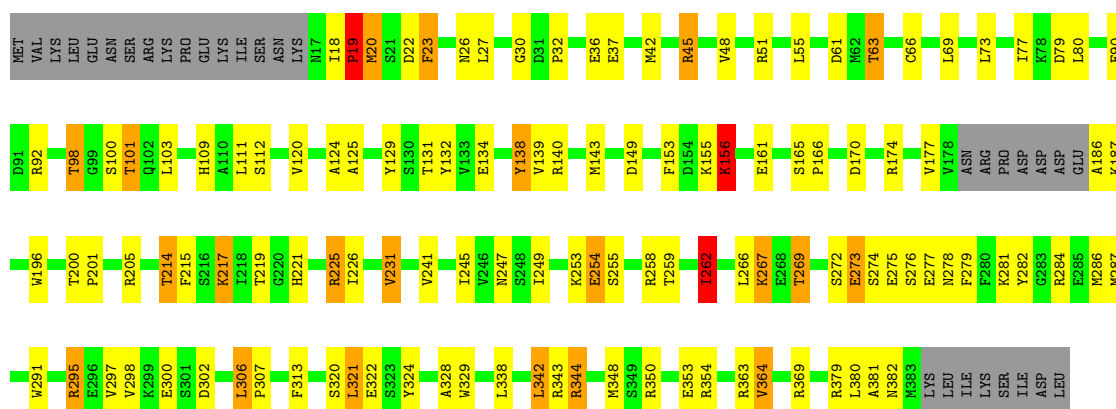
• Molecule 1: L-tryptophan aminotransferase





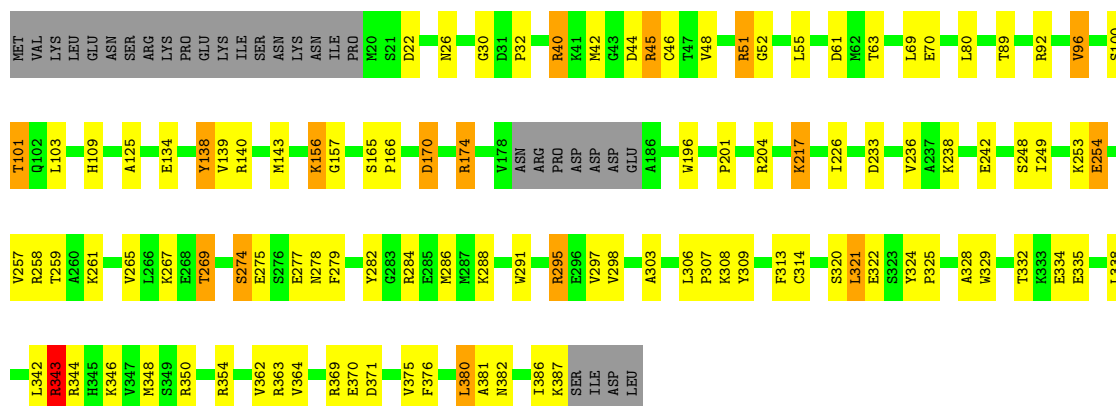
• Molecule 1: L-tryptophan aminotransferase

Chain D: 60% 26% 5% • 8%



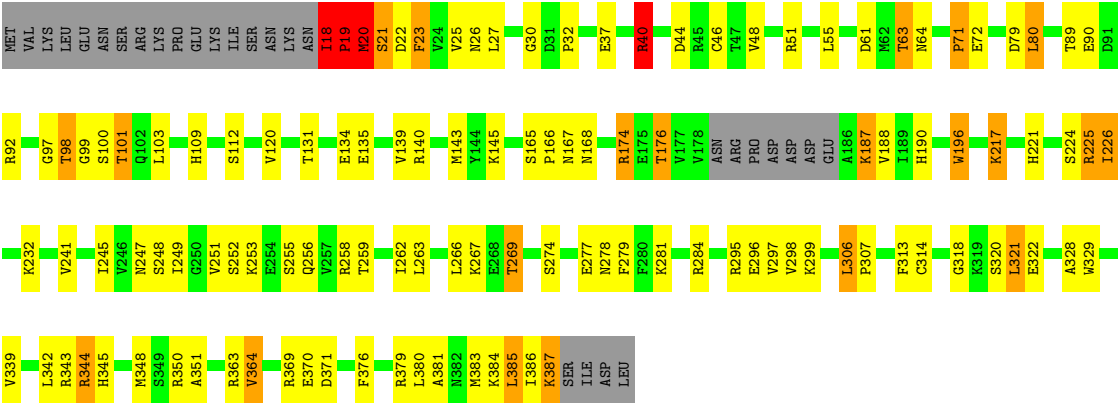
• Molecule 1: L-tryptophan aminotransferase

Chain E: 65% 23% • 8%



• Molecule 1: L-tryptophan aminotransferase

Chain F: 62% 24% 5% • 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.33Å 98.66Å 139.36Å 90.00° 104.50° 90.00°	Depositor
Resolution (Å)	29.66 – 2.40 29.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.66-2.40) 98.0 (29.66-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.238 , 0.253 0.238 , 0.253	Depositor DCC
R_{free} test set	4682 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18479	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0544e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.82	1/2979 (0.0%)	1.00	9/4025 (0.2%)
1	B	0.86	6/2987 (0.2%)	1.03	5/4036 (0.1%)
1	C	0.81	2/2954 (0.1%)	1.03	9/3992 (0.2%)
1	D	0.83	7/2953 (0.2%)	1.03	11/3992 (0.3%)
1	E	0.80	5/2963 (0.2%)	1.02	12/4002 (0.3%)
1	F	0.97	13/2979 (0.4%)	1.10	20/4025 (0.5%)
All	All	0.85	34/17815 (0.2%)	1.03	66/24072 (0.3%)

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	D	0	1
1	F	0	2
All	All	0	3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	344	ARG	NE-CZ	14.17	1.48	1.33
1	F	140	ARG	CZ-NH2	-11.92	1.18	1.33
1	F	40	ARG	CD-NE	10.80	1.61	1.46
1	D	23	PHE	C-N	-10.00	1.21	1.33
1	F	19	PRO	N-CD	8.70	1.59	1.47
1	F	23	PHE	CA-C	-8.60	1.42	1.52
1	E	343	ARG	NE-CZ	8.56	1.42	1.33
1	F	19	PRO	N-CA	7.81	1.57	1.47
1	F	344	ARG	CZ-NH2	-7.57	1.23	1.33
1	F	344	ARG	CD-NE	-7.55	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	343	ARG	CZ-NH2	7.50	1.43	1.33
1	A	116	ARG	CZ-NH2	-6.95	1.24	1.33
1	B	287	MET	SD-CE	-6.93	1.62	1.79
1	D	287	MET	SD-CE	-6.66	1.62	1.79
1	B	156	LYS	CB-CG	6.49	1.72	1.52
1	F	21	SER	CA-C	6.34	1.61	1.52
1	C	354	ARG	CZ-NH2	-6.31	1.25	1.33
1	F	19	PRO	C-O	6.24	1.32	1.24
1	D	273	GLU	CD-OE1	6.08	1.36	1.25
1	F	21	SER	C-N	-6.02	1.25	1.33
1	F	343	ARG	CZ-NH2	-5.89	1.25	1.33
1	D	262	ILE	CB-CG2	-5.89	1.33	1.52
1	B	151	TRP	C-O	-5.85	1.16	1.24
1	D	156	LYS	CE-NZ	-5.83	1.31	1.49
1	C	116	ARG	CG-CD	5.65	1.69	1.52
1	E	51	ARG	NE-CZ	-5.50	1.27	1.33
1	D	262	ILE	CG1-CD1	-5.45	1.30	1.51
1	B	40	ARG	CZ-NH1	-5.41	1.25	1.32
1	F	19	PRO	CA-CB	5.40	1.61	1.53
1	E	343	ARG	CZ-NH1	-5.30	1.25	1.32
1	E	70	GLU	C-N	-5.26	1.26	1.33
1	B	96	VAL	CA-CB	5.21	1.61	1.54
1	D	262	ILE	CB-CG1	-5.15	1.43	1.53
1	B	226	ILE	CA-CB	5.06	1.61	1.54

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	18	ILE	CA-C-N	15.38	139.07	119.84
1	F	18	ILE	C-N-CA	15.38	139.07	119.84
1	C	354	ARG	NE-CZ-NH2	13.09	130.98	119.20
1	E	343	ARG	NE-CZ-NH2	12.44	130.40	119.20
1	F	140	ARG	NE-CZ-NH2	9.89	128.10	119.20
1	F	385	LEU	N-CA-C	-9.58	90.39	110.80
1	E	51	ARG	NE-CZ-NH2	-8.26	111.77	119.20
1	D	23	PHE	O-C-N	-7.81	114.15	123.13
1	C	354	ARG	NH1-CZ-NH2	-7.70	109.29	119.30
1	B	40	ARG	NE-CZ-NH2	7.47	125.92	119.20
1	F	40	ARG	CD-NE-CZ	-7.38	114.07	124.40
1	A	116	ARG	NE-CZ-NH2	7.34	125.80	119.20
1	F	20	MET	CA-C-N	-7.24	107.72	121.54
1	F	20	MET	C-N-CA	-7.24	107.72	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	196	TRP	CA-C-N	7.16	126.69	119.24
1	C	196	TRP	C-N-CA	7.16	126.69	119.24
1	E	40	ARG	NE-CZ-NH2	7.01	125.51	119.20
1	D	354	ARG	NE-CZ-NH2	6.98	125.48	119.20
1	B	138	TYR	N-CA-C	6.92	119.67	111.71
1	E	274	SER	N-CA-C	-6.80	97.51	109.06
1	D	276	SER	N-CA-C	-6.68	105.04	113.72
1	D	262	ILE	CB-CG1-CD1	-6.63	99.88	113.80
1	B	40	ARG	NE-CZ-NH1	-6.58	114.92	121.50
1	A	116	ARG	CD-NE-CZ	-6.52	115.28	124.40
1	D	354	ARG	NE-CZ-NH1	-6.42	115.08	121.50
1	F	23	PHE	CA-CB-CG	6.31	120.11	113.80
1	F	23	PHE	N-CA-CB	6.25	120.75	110.69
1	E	138	TYR	N-CA-C	6.25	119.75	111.75
1	E	96	VAL	CB-CA-C	-6.20	102.44	111.68
1	A	23	PHE	CD1-CG-CD2	-6.19	109.32	118.60
1	B	262	ILE	CB-CG1-CD1	-6.10	101.00	113.80
1	F	168	ASN	N-CA-C	-6.06	100.18	109.64
1	F	369	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	F	344	ARG	NE-CZ-NH1	6.05	127.55	121.50
1	D	196	TRP	CA-C-N	5.97	126.40	119.47
1	D	196	TRP	C-N-CA	5.97	126.40	119.47
1	C	212	LEU	CD1-CG-CD2	-5.89	97.83	110.80
1	F	23	PHE	N-CA-C	5.86	119.03	109.59
1	A	23	PHE	CB-CG-CD1	5.79	130.54	120.70
1	A	138	TYR	N-CA-C	5.72	119.08	111.75
1	A	276	SER	N-CA-C	-5.70	106.67	113.97
1	E	196	TRP	CA-C-N	5.69	126.08	119.47
1	E	196	TRP	C-N-CA	5.69	126.08	119.47
1	F	71	PRO	O-C-N	-5.63	115.03	122.64
1	C	369	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	F	140	ARG	NH1-CZ-NH2	-5.52	112.12	119.30
1	F	226	ILE	N-CA-C	5.51	115.93	107.77
1	A	321	LEU	N-CA-C	5.48	117.31	109.14
1	D	138	TYR	N-CA-C	5.45	119.43	112.34
1	E	170	ASP	N-CA-C	5.44	119.66	113.19
1	C	321	LEU	CD1-CG-CD2	-5.42	98.87	110.80
1	B	369	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	C	273	GLU	CB-CA-C	-5.32	102.08	110.86
1	A	96	VAL	CB-CA-C	-5.30	103.97	111.38
1	E	343	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	D	369	ARG	NE-CZ-NH2	5.26	123.93	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	45	ARG	N-CA-CB	-5.24	101.70	110.39
1	F	18	ILE	C-N-CD	-5.21	103.63	125.00
1	F	196	TRP	CA-C-N	5.21	125.52	119.47
1	F	196	TRP	C-N-CA	5.21	125.52	119.47
1	D	300	GLU	CB-CA-C	-5.10	99.80	109.95
1	E	174	ARG	N-CA-C	5.08	117.13	109.41
1	F	174	ARG	N-CA-C	5.04	117.33	109.52
1	C	174	ARG	N-CA-C	5.04	117.51	109.81
1	A	369	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	D	262	ILE	CG1-CB-CG2	-5.00	95.69	110.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	19	PRO	Peptide
1	F	18	ILE	Peptide
1	F	19	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	2935	0	2862	79	0
1	B	2943	0	2878	97	0
1	C	2910	0	2838	95	0
1	D	2909	0	2830	99	0
1	E	2920	0	2855	93	0
1	F	2935	0	2873	122	0
2	A	161	0	0	4	0
2	B	184	0	0	20	0
2	C	132	0	0	7	0
2	D	159	0	0	11	0
2	E	135	0	0	8	0
2	F	156	0	0	15	0
All	All	18479	0	17136	553	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 16.

All (553) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:LYS:HB2	1:E:156:LYS:NZ	1.57	1.12
1:B:344:ARG:HH11	1:B:344:ARG:HB2	1.09	1.12
1:F:386:ILE:HG22	1:F:387:LYS:H	1.13	1.07
1:F:385:LEU:HB3	1:F:386:ILE:HD12	1.40	1.02
1:F:20:MET:HG2	1:F:21:SER:N	1.72	1.02
1:B:386:ILE:HG21	2:B:411:HOH:O	1.59	1.01
1:F:274:SER:HB3	1:F:277:GLU:HB2	1.43	0.97
1:E:156:LYS:NZ	1:E:156:LYS:CB	2.29	0.95
1:A:156:LYS:HD3	1:A:156:LYS:H	1.26	0.95
1:E:156:LYS:HB2	1:E:156:LYS:HZ2	1.20	0.95
1:F:344:ARG:HE	1:F:387:LYS:HE3	1.32	0.94
1:A:344:ARG:HB3	1:A:344:ARG:NH1	1.84	0.92
1:D:274:SER:HB3	1:D:277:GLU:HB2	1.49	0.91
1:C:186:ALA:N	2:C:521:HOH:O	2.03	0.90
1:C:274:SER:HB3	1:C:277:GLU:HB2	1.54	0.90
1:F:20:MET:O	1:F:21:SER:CB	2.18	0.89
1:E:156:LYS:HG3	1:E:157:GLY:N	1.88	0.89
1:F:20:MET:HG2	1:F:21:SER:H	1.36	0.88
1:F:20:MET:CG	1:F:21:SER:H	1.87	0.88
1:B:274:SER:HB3	1:B:277:GLU:HB2	1.53	0.88
1:B:344:ARG:HB2	1:B:344:ARG:NH1	1.88	0.88
1:A:69:LEU:HD13	1:A:96:VAL:HG13	1.55	0.87
1:D:284:ARG:NH2	1:D:322:GLU:O	2.06	0.87
1:F:328:ALA:HB3	1:F:364:VAL:HG13	1.56	0.87
1:A:274:SER:HB3	1:A:277:GLU:HB2	1.53	0.87
1:E:297:VAL:HG23	2:E:524:HOH:O	1.75	0.87
1:A:156:LYS:HD3	1:A:156:LYS:N	1.89	0.86
1:E:274:SER:HB3	1:E:277:GLU:HB2	1.58	0.86
1:F:226:ILE:HD13	2:F:478:HOH:O	1.74	0.86
1:F:20:MET:C	1:F:22:ASP:H	1.85	0.85
1:A:328:ALA:HB3	1:A:364:VAL:HG13	1.58	0.84
1:A:284:ARG:NH2	1:A:322:GLU:O	2.09	0.83
1:F:20:MET:CG	1:F:21:SER:N	2.39	0.83
1:A:16:LYS:HG3	1:A:17:ASN:H	1.44	0.82
1:B:156:LYS:H	1:B:156:LYS:HD3	1.44	0.81
1:F:386:ILE:HG22	1:F:387:LYS:N	1.96	0.81
1:E:109:HIS:CD2	1:E:143:MET:HE1	2.15	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:LYS:HB2	1:E:156:LYS:HZ1	1.46	0.80
1:F:20:MET:O	1:F:21:SER:OG	1.99	0.80
1:E:156:LYS:HZ1	1:E:156:LYS:HA	1.46	0.79
1:F:298:VAL:HG21	1:F:306:LEU:HD22	1.65	0.79
1:D:18:ILE:HD11	1:D:23:PHE:HZ	1.48	0.79
1:A:269:THR:HG23	1:A:278:ASN:HA	1.63	0.78
1:E:284:ARG:NH2	1:E:322:GLU:O	2.16	0.78
1:E:156:LYS:HZ1	1:E:156:LYS:CA	1.96	0.78
1:E:156:LYS:CB	1:E:156:LYS:HZ1	1.96	0.78
1:A:217:LLP:H4'1	2:A:492:HOH:O	1.84	0.77
1:B:387:LYS:HE3	2:B:574:HOH:O	1.83	0.77
1:C:109:HIS:ND1	1:C:143:MET:HE1	2.00	0.76
1:B:328:ALA:HB3	1:B:364:VAL:HG13	1.68	0.76
1:B:109:HIS:CD2	1:B:143:MET:HE1	2.20	0.75
1:B:312:ALA:HB2	2:B:530:HOH:O	1.86	0.75
1:C:48:VAL:HG21	1:C:258:ARG:HG3	1.69	0.75
1:B:275:GLU:HG3	1:B:281:LYS:HD2	1.69	0.74
1:D:328:ALA:HB3	1:D:364:VAL:HG13	1.70	0.74
1:E:298:VAL:HG21	1:E:306:LEU:HD22	1.70	0.73
1:D:344:ARG:HH11	1:D:344:ARG:HG2	1.54	0.73
1:A:269:THR:CG2	1:A:279:PHE:H	2.02	0.73
1:A:297:VAL:HG13	1:A:381:ALA:HB2	1.69	0.72
1:A:247:ASN:ND2	2:A:466:HOH:O	2.23	0.72
1:A:344:ARG:HB3	1:A:344:ARG:HH11	1.54	0.71
1:B:287:MET:SD	2:B:503:HOH:O	2.47	0.71
1:C:383:MET:O	1:C:384:LYS:HD2	1.90	0.71
1:F:284:ARG:NH2	1:F:322:GLU:O	2.23	0.70
1:D:100:SER:N	1:D:217:LLP:OP2	2.24	0.70
1:E:269:THR:CG2	1:E:279:PHE:H	2.04	0.70
1:E:344:ARG:NH1	1:E:344:ARG:HB3	2.05	0.70
1:B:156:LYS:HD3	1:B:156:LYS:N	2.06	0.70
1:F:344:ARG:HH11	1:F:344:ARG:HG2	1.55	0.69
1:C:328:ALA:HB3	1:C:364:VAL:HG13	1.73	0.69
1:D:379:ARG:NH2	2:D:532:HOH:O	2.24	0.69
1:B:161:GLU:OE1	1:B:178:VAL:HG12	1.92	0.69
1:F:344:ARG:NE	1:F:387:LYS:HE3	2.06	0.69
1:E:51:ARG:NH1	2:E:499:HOH:O	2.25	0.69
1:C:343:ARG:HG3	1:C:348:MET:HE1	1.74	0.68
1:F:79:ASP:HB3	1:F:267:LYS:HE2	1.76	0.68
1:A:70:GLU:HG3	1:A:72:GLU:OE1	1.94	0.68
1:B:384:LYS:H	1:B:387:LYS:NZ	1.91	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:THR:HG21	1:A:279:PHE:H	1.59	0.67
1:E:297:VAL:HG13	1:E:381:ALA:HB2	1.76	0.67
1:B:298:VAL:HG21	1:B:306:LEU:HD22	1.74	0.67
1:B:344:ARG:HH11	1:B:344:ARG:CB	1.98	0.67
1:A:100:SER:N	1:A:217:LLP:OP2	2.27	0.67
1:D:101:THR:HB	2:D:502:HOH:O	1.95	0.67
1:B:198:HIS:HA	1:B:284:ARG:HG3	1.77	0.67
1:F:386:ILE:CG2	1:F:387:LYS:H	1.94	0.67
1:B:55:LEU:HD13	1:B:253:LYS:HB3	1.77	0.66
1:C:249:ILE:CD1	1:D:101:THR:HG21	2.25	0.66
1:E:254:GLU:OE2	1:F:258:ARG:HD3	1.95	0.66
1:D:20:MET:HG3	1:D:23:PHE:CD1	2.30	0.66
1:A:69:LEU:HD13	1:A:96:VAL:CG1	2.25	0.66
1:F:61:ASP:OD1	1:F:63:THR:HB	1.96	0.66
1:C:297:VAL:HG13	1:C:381:ALA:HB2	1.78	0.66
1:C:141:SER:HB2	1:D:139:VAL:O	1.95	0.66
1:F:344:ARG:HE	1:F:387:LYS:CE	2.08	0.66
1:D:269:THR:HG23	1:D:278:ASN:HA	1.78	0.66
1:D:281:LYS:HD3	1:D:281:LYS:C	2.21	0.65
1:F:385:LEU:HD23	1:F:386:ILE:HD11	1.77	0.65
1:C:100:SER:N	1:C:217:LLP:OP2	2.30	0.65
1:F:345:HIS:ND1	2:F:504:HOH:O	2.23	0.65
1:C:226:ILE:HG21	1:C:259:THR:HG21	1.77	0.65
1:F:100:SER:N	1:F:217:LLP:OP2	2.30	0.64
1:F:385:LEU:HB3	1:F:386:ILE:CD1	2.23	0.64
1:E:45:ARG:NH1	1:E:265:VAL:HG13	2.12	0.64
1:D:219:THR:HG21	1:D:262:ILE:HD11	1.80	0.64
1:F:269:THR:CG2	1:F:279:PHE:H	2.10	0.64
1:A:61:ASP:OD1	1:A:63:THR:HB	1.98	0.64
1:B:217:LLP:H4'1	2:B:486:HOH:O	1.98	0.64
1:B:313:PHE:HA	1:B:320:SER:HA	1.80	0.63
1:F:386:ILE:HG12	2:F:408:HOH:O	1.96	0.63
1:F:187:LYS:HE3	2:F:520:HOH:O	1.97	0.63
1:F:226:ILE:HA	2:F:478:HOH:O	1.99	0.62
1:D:61:ASP:OD1	1:D:63:THR:HB	1.99	0.62
1:B:269:THR:CG2	1:B:279:PHE:H	2.11	0.62
1:D:344:ARG:HH11	1:D:344:ARG:CG	2.12	0.62
1:E:55:LEU:HD13	1:E:253:LYS:HB3	1.81	0.62
1:B:384:LYS:H	1:B:387:LYS:HZ3	1.48	0.62
1:C:61:ASP:OD1	1:C:63:THR:HB	2.00	0.62
1:D:215:PHE:HZ	1:D:262:ILE:HG12	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:SER:HA	1:B:254:GLU:OE1	2.00	0.61
1:B:100:SER:N	1:B:217:LLP:OP2	2.34	0.61
1:C:101:THR:HG21	1:D:249:ILE:CD1	2.30	0.61
1:E:69:LEU:HD13	1:E:96:VAL:HG13	1.81	0.61
1:C:175:GLU:HG3	2:C:484:HOH:O	2.01	0.61
1:A:241:VAL:O	1:A:245:ILE:HG13	2.01	0.61
1:F:252:SER:HB3	2:F:403:HOH:O	2.00	0.61
1:D:266:LEU:O	1:D:269:THR:HB	2.01	0.60
1:F:344:ARG:HH21	1:F:387:LYS:NZ	1.99	0.60
1:D:18:ILE:HD11	1:D:23:PHE:CZ	2.32	0.60
1:E:284:ARG:NH2	1:E:321:LEU:HG	2.17	0.60
1:C:298:VAL:HG21	1:C:306:LEU:HD22	1.83	0.59
1:A:64:ASN:HB3	2:A:512:HOH:O	2.02	0.59
1:D:295:ARG:NH2	1:D:307:PRO:O	2.33	0.59
1:E:284:ARG:HH21	1:E:321:LEU:HG	1.67	0.59
1:B:320:SER:HB2	2:B:423:HOH:O	2.02	0.59
1:D:98:THR:HB	2:D:402:HOH:O	2.02	0.59
1:C:335:GLU:OE2	1:C:360:LYS:HE2	2.03	0.59
1:F:269:THR:HG23	1:F:278:ASN:HA	1.84	0.59
1:E:48:VAL:HG21	1:E:258:ARG:HG3	1.83	0.59
1:F:307:PRO:HG2	1:F:329:TRP:HB3	1.85	0.59
1:B:278:ASN:OD1	2:B:407:HOH:O	2.16	0.59
1:E:328:ALA:HB3	1:E:364:VAL:HG13	1.85	0.59
1:F:344:ARG:HH21	1:F:387:LYS:HZ3	1.51	0.59
1:F:109:HIS:ND1	1:F:143:MET:HE1	2.18	0.59
1:D:269:THR:CG2	1:D:279:PHE:H	2.16	0.58
1:B:139:VAL:HG22	2:B:401:HOH:O	2.02	0.58
1:A:109:HIS:CD2	1:A:143:MET:HE1	2.39	0.58
1:F:26:ASN:HA	1:F:348:MET:HB2	1.85	0.58
1:D:139:VAL:HG22	2:D:397:HOH:O	2.02	0.58
1:B:48:VAL:HG21	1:B:258:ARG:HG3	1.85	0.58
1:C:266:LEU:O	1:C:269:THR:HG22	2.04	0.58
1:C:346:LYS:HB2	1:C:379:ARG:NH1	2.19	0.58
1:D:79:ASP:HB3	1:D:267:LYS:HE3	1.84	0.58
1:E:238:LYS:O	1:E:242:GLU:HG3	2.04	0.58
1:A:344:ARG:HH11	1:A:344:ARG:CB	2.17	0.58
1:C:109:HIS:HE1	1:D:138:TYR:O	1.86	0.58
1:C:40:ARG:HD2	2:C:467:HOH:O	2.04	0.57
1:C:344:ARG:HH11	1:C:344:ARG:HB3	1.68	0.57
1:F:64:ASN:HB3	2:F:416:HOH:O	2.04	0.57
1:D:186:ALA:O	1:D:187:LYS:HD3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:ILE:HG21	1:E:259:THR:HG21	1.86	0.57
1:F:241:VAL:O	1:F:245:ILE:HG13	2.05	0.57
1:E:350:ARG:HB3	1:E:363:ARG:HB3	1.85	0.57
1:B:262:ILE:HG13	1:B:263:LEU:N	2.19	0.56
1:F:98:THR:HG22	2:F:406:HOH:O	2.04	0.56
1:B:225:ARG:HA	1:B:225:ARG:NE	2.20	0.56
1:D:109:HIS:HE2	1:D:143:MET:HE1	1.70	0.56
1:B:345:HIS:NE2	1:B:387:LYS:HD3	2.20	0.56
1:E:269:THR:HG23	1:E:278:ASN:HA	1.85	0.56
1:C:307:PRO:HG2	1:C:329:TRP:HB3	1.88	0.56
1:A:109:HIS:NE2	1:A:143:MET:HE1	2.21	0.56
1:C:18:ILE:N	1:C:19:PRO:HD2	2.20	0.56
1:F:18:ILE:HG22	1:F:18:ILE:O	2.06	0.56
1:F:176:THR:HG21	1:F:188:VAL:HG21	1.87	0.55
1:D:217:LLP:P	1:D:225:ARG:HH22	2.29	0.55
1:A:226:ILE:HG21	1:A:259:THR:HG21	1.88	0.55
1:E:303:ALA:O	1:E:332:THR:HA	2.06	0.55
1:A:101:THR:HG21	1:B:249:ILE:CD1	2.35	0.55
1:C:344:ARG:HH11	1:C:344:ARG:CG	2.19	0.55
1:E:42:MET:HE3	1:E:45:ARG:HD3	1.89	0.55
1:F:109:HIS:CE1	1:F:143:MET:HE1	2.42	0.55
1:C:381:ALA:C	1:C:382:ASN:HD22	2.15	0.54
1:D:298:VAL:HG21	1:D:306:LEU:HD22	1.88	0.54
1:D:284:ARG:HH21	1:D:321:LEU:HG	1.73	0.54
1:C:45:ARG:HH11	1:C:265:VAL:HG13	1.73	0.54
1:C:284:ARG:NH2	1:C:321:LEU:HD13	2.23	0.54
1:D:217:LLP:H4'1	2:D:464:HOH:O	2.06	0.54
1:F:225:ARG:CZ	1:F:225:ARG:HA	2.38	0.54
1:A:282:TYR:CE1	1:A:286:MET:HE3	2.42	0.54
1:A:284:ARG:NH2	1:A:321:LEU:HG	2.23	0.54
1:D:225:ARG:HA	1:D:225:ARG:NE	2.22	0.54
1:F:344:ARG:HG2	1:F:344:ARG:NH1	2.17	0.54
1:E:156:LYS:CG	1:E:157:GLY:N	2.66	0.53
1:A:89:THR:HA	1:A:92:ARG:HD2	1.89	0.53
1:F:350:ARG:HB3	1:F:363:ARG:HB3	1.90	0.53
1:B:61:ASP:OD1	1:B:63:THR:HB	2.08	0.53
1:F:344:ARG:NE	1:F:387:LYS:CE	2.69	0.53
1:C:217:LLP:OP3	1:D:249:ILE:HD12	2.08	0.53
1:B:282:TYR:CE1	1:B:286:MET:HE3	2.43	0.53
1:D:124:ALA:O	1:D:149:ASP:HA	2.08	0.53
1:F:20:MET:HG3	1:F:21:SER:H	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LLP:P	1:B:225:ARG:HH22	2.32	0.53
1:B:269:THR:HG23	1:B:279:PHE:H	1.72	0.53
1:C:139:VAL:HG22	2:C:446:HOH:O	2.08	0.53
1:E:101:THR:HG21	1:F:249:ILE:CD1	2.39	0.53
1:F:269:THR:HG21	1:F:279:PHE:H	1.74	0.53
1:C:18:ILE:N	1:C:19:PRO:CD	2.72	0.53
1:C:55:LEU:HB3	1:C:253:LYS:HG2	1.90	0.53
1:C:109:HIS:CE1	1:C:143:MET:HE1	2.43	0.53
1:E:217:LLP:H4'1	2:E:463:HOH:O	2.09	0.53
1:A:350:ARG:HB3	1:A:363:ARG:HB3	1.90	0.53
1:C:42:MET:HE3	1:C:45:ARG:HD2	1.89	0.53
1:D:48:VAL:HG21	1:D:258:ARG:HG3	1.90	0.53
1:E:295:ARG:NH2	1:E:307:PRO:O	2.40	0.53
1:E:45:ARG:HH11	1:E:265:VAL:HG13	1.73	0.52
1:B:386:ILE:HD13	2:B:411:HOH:O	2.08	0.52
1:F:297:VAL:HG13	1:F:381:ALA:HB2	1.91	0.52
1:D:129:TYR:CZ	1:D:131:THR:HB	2.43	0.52
1:D:262:ILE:C	1:D:262:ILE:HD12	2.34	0.52
1:E:140:ARG:HD3	1:F:143:MET:HG2	1.90	0.52
1:E:282:TYR:CE1	1:E:286:MET:HE3	2.44	0.52
1:C:116:ARG:H	1:C:116:ARG:HE	1.57	0.52
1:C:326:ALA:HB1	1:C:367:LEU:HD11	1.92	0.52
1:A:55:LEU:HD13	1:A:253:LYS:HB3	1.91	0.52
1:E:308:LYS:HG2	2:E:483:HOH:O	2.08	0.52
1:B:225:ARG:HA	1:B:225:ARG:CZ	2.40	0.52
1:B:307:PRO:HG2	1:B:329:TRP:HB3	1.92	0.52
1:C:30:GLY:O	1:C:32:PRO:HD3	2.10	0.52
1:E:249:ILE:HG13	1:F:101:THR:HG21	1.90	0.52
1:C:80:LEU:HD13	1:C:196:TRP:CH2	2.45	0.52
1:D:156:LYS:H	1:D:156:LYS:HD2	1.75	0.51
1:E:89:THR:HA	1:E:92:ARG:HD2	1.91	0.51
1:F:281:LYS:C	1:F:281:LYS:HD3	2.35	0.51
1:C:111:LEU:HD13	1:C:187:LYS:HB3	1.92	0.51
1:C:344:ARG:CG	1:C:344:ARG:NH1	2.69	0.51
1:A:285:GLU:CB	2:A:455:HOH:O	2.59	0.51
1:C:249:ILE:HG13	1:D:101:THR:HG21	1.91	0.51
1:A:344:ARG:HB3	1:A:344:ARG:CZ	2.41	0.51
1:F:98:THR:HG22	1:F:251:VAL:HG13	1.93	0.51
1:F:101:THR:HG22	1:F:217:LLP:OP2	2.10	0.51
1:B:269:THR:HG21	1:B:279:PHE:H	1.76	0.51
1:C:344:ARG:NH1	1:C:344:ARG:HG2	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:PHE:HA	1:D:320:SER:HA	1.93	0.51
1:F:321:LEU:N	1:F:321:LEU:CD2	2.74	0.51
1:A:44:ASP:CG	1:B:51:ARG:HH22	2.19	0.51
1:B:55:LEU:HD11	1:B:257:VAL:HG21	1.91	0.51
1:B:97:GLY:O	1:B:99:GLY:N	2.44	0.51
1:F:296:GLU:O	1:F:299:LYS:HB3	2.11	0.51
1:C:40:ARG:HG3	1:C:40:ARG:HH11	1.76	0.51
1:E:344:ARG:HH11	1:E:344:ARG:CB	2.24	0.50
1:A:338:LEU:O	1:A:342:LEU:HB2	2.10	0.50
1:C:101:THR:HG21	1:D:249:ILE:HD11	1.93	0.50
1:C:344:ARG:HH11	1:C:344:ARG:CB	2.24	0.50
1:D:291:TRP:O	1:D:295:ARG:HB2	2.11	0.50
1:E:313:PHE:HA	1:E:320:SER:HA	1.93	0.50
2:E:499:HOH:O	1:F:44:ASP:CG	2.55	0.50
1:F:97:GLY:O	1:F:99:GLY:N	2.45	0.50
1:B:328:ALA:HA	2:B:483:HOH:O	2.12	0.50
1:C:61:ASP:CG	1:C:63:THR:HB	2.37	0.50
1:C:335:GLU:O	1:C:336:THR:HG23	2.11	0.50
1:E:26:ASN:HA	1:E:348:MET:HB2	1.94	0.50
1:E:344:ARG:NH1	1:E:344:ARG:CB	2.72	0.50
1:A:291:TRP:CD1	1:A:324:TYR:HB3	2.46	0.50
1:B:165:SER:HA	1:B:166:PRO:C	2.36	0.50
1:D:282:TYR:CE1	1:D:286:MET:HE3	2.47	0.50
1:C:226:ILE:HG13	1:C:259:THR:OG1	2.12	0.50
1:E:143:MET:HE2	1:F:139:VAL:HA	1.93	0.50
1:B:98:THR:HG22	2:B:406:HOH:O	2.11	0.50
1:C:89:THR:HA	1:C:92:ARG:HD2	1.94	0.50
1:D:30:GLY:O	1:D:32:PRO:HD3	2.12	0.50
1:E:291:TRP:O	1:E:295:ARG:HB2	2.12	0.49
1:C:284:ARG:CZ	1:C:321:LEU:HD13	2.42	0.49
1:F:25:VAL:HG11	1:F:376:PHE:HB2	1.93	0.49
1:B:296:GLU:O	1:B:299:LYS:HB3	2.12	0.49
1:C:252:SER:O	1:C:256:GLN:HG3	2.12	0.49
1:F:48:VAL:HG21	1:F:258:ARG:HG3	1.93	0.49
1:F:251:VAL:HG11	2:F:478:HOH:O	2.13	0.49
1:C:208:HIS:O	1:C:232:LYS:HE2	2.12	0.49
1:A:80:LEU:HD12	1:A:196:TRP:CZ3	2.48	0.49
1:B:42:MET:HE3	1:B:45:ARG:HD3	1.93	0.49
1:E:100:SER:N	1:E:217:LLP:OP2	2.44	0.49
1:E:288:LYS:HG3	1:E:324:TYR:CZ	2.47	0.49
1:C:295:ARG:NH2	1:C:307:PRO:O	2.35	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ASN:HA	1:D:348:MET:HB2	1.95	0.49
1:E:249:ILE:HD12	1:F:217:LLP:OP3	2.13	0.49
1:A:30:GLY:O	1:A:32:PRO:HD3	2.13	0.49
1:D:200:THR:OG1	1:D:201:PRO:HD2	2.13	0.49
1:F:269:THR:HG23	1:F:279:PHE:H	1.76	0.49
1:F:284:ARG:NH2	1:F:321:LEU:HG	2.28	0.49
1:F:344:ARG:HB3	1:F:387:LYS:HE2	1.94	0.49
1:A:200:THR:OG1	1:A:201:PRO:HD2	2.13	0.48
1:E:22:ASP:HA	1:E:346:LYS:NZ	2.28	0.48
1:E:254:GLU:OE1	1:F:224:SER:HA	2.13	0.48
1:E:307:PRO:HG2	1:E:329:TRP:HB3	1.94	0.48
1:B:64:ASN:HB3	2:B:421:HOH:O	2.12	0.48
1:E:344:ARG:HB3	1:E:344:ARG:CZ	2.43	0.48
1:F:321:LEU:N	1:F:321:LEU:HD23	2.28	0.48
1:C:326:ALA:HB1	1:C:367:LEU:CD1	2.43	0.48
1:D:112:SER:HA	1:D:120:VAL:HG21	1.94	0.48
1:C:354:ARG:HG2	1:C:354:ARG:HH11	1.79	0.48
1:A:169:PRO:HB3	1:A:363:ARG:HD3	1.96	0.48
1:E:40:ARG:HG3	1:E:40:ARG:HH11	1.79	0.48
1:D:344:ARG:CZ	1:D:344:ARG:HB3	2.43	0.48
1:C:45:ARG:NE	2:C:518:HOH:O	2.47	0.48
1:C:129:TYR:HB3	1:C:132:TYR:CD2	2.48	0.48
1:D:350:ARG:HB3	1:D:363:ARG:HB3	1.96	0.48
1:D:27:LEU:HD13	1:D:364:VAL:HG23	1.95	0.48
1:F:30:GLY:O	1:F:32:PRO:HD3	2.14	0.47
1:B:221:HIS:CE1	1:B:262:ILE:HD13	2.49	0.47
1:F:386:ILE:HD12	1:F:386:ILE:N	2.29	0.47
1:D:100:SER:HB2	1:D:214:THR:HB	1.96	0.47
1:D:231:VAL:HG12	2:D:460:HOH:O	2.15	0.47
1:F:221:HIS:CE1	1:F:262:ILE:HD13	2.49	0.47
1:F:55:LEU:HB3	1:F:253:LYS:HB3	1.95	0.47
1:F:383:MET:O	1:F:384:LYS:C	2.57	0.47
1:B:174:ARG:HB3	2:B:415:HOH:O	2.15	0.47
1:D:344:ARG:CG	1:D:344:ARG:NH1	2.74	0.47
1:A:354:ARG:HG2	1:A:354:ARG:HH11	1.78	0.47
1:B:167:ASN:HB2	1:B:174:ARG:HD2	1.96	0.47
1:B:226:ILE:HG21	1:B:259:THR:HG21	1.97	0.47
1:E:30:GLY:O	1:E:32:PRO:HD3	2.14	0.47
1:F:165:SER:HA	1:F:166:PRO:C	2.39	0.47
1:B:98:THR:HG22	1:B:251:VAL:HG13	1.97	0.47
1:C:269:THR:CG2	1:C:279:PHE:H	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LEU:HB3	1:D:253:LYS:HB3	1.96	0.47
1:E:321:LEU:N	1:E:321:LEU:CD2	2.77	0.47
1:B:30:GLY:O	1:B:32:PRO:HD3	2.15	0.47
1:E:165:SER:HA	1:E:166:PRO:C	2.40	0.47
1:A:321:LEU:N	1:A:321:LEU:CD2	2.78	0.46
1:C:18:ILE:HG13	1:C:19:PRO:HD3	1.97	0.46
1:D:66:CYS:SG	1:D:69:LEU:HB2	2.56	0.46
1:E:354:ARG:HG2	1:E:354:ARG:HH11	1.79	0.46
1:A:298:VAL:HG21	1:A:306:LEU:HD22	1.95	0.46
1:B:112:SER:HA	1:B:120:VAL:HG21	1.97	0.46
1:D:111:LEU:HD22	1:D:187:LYS:HG3	1.97	0.46
1:A:80:LEU:CD1	1:A:196:TRP:CZ3	2.99	0.46
1:C:170:ASP:HA	1:C:329:TRP:HB2	1.97	0.46
1:D:19:PRO:HG3	1:D:22:ASP:HB2	1.97	0.46
1:D:297:VAL:HG13	1:D:381:ALA:HB2	1.96	0.46
1:B:284:ARG:NH2	1:B:321:LEU:HG	2.31	0.46
1:E:269:THR:HG21	1:E:279:PHE:H	1.77	0.46
1:E:44:ASP:CG	1:F:51:ARG:HH22	2.24	0.46
1:F:314:CYS:HB2	1:F:321:LEU:HD21	1.98	0.46
1:E:48:VAL:HG21	1:E:258:ARG:HA	1.97	0.46
1:A:295:ARG:NH2	1:A:307:PRO:O	2.49	0.46
1:B:344:ARG:HH21	1:B:387:LYS:HB3	1.81	0.46
1:E:309:TYR:CZ	1:E:325:PRO:HG2	2.51	0.46
1:A:156:LYS:H	1:A:156:LYS:CD	2.12	0.46
1:D:321:LEU:N	1:D:321:LEU:CD2	2.79	0.46
1:E:303:ALA:CB	1:E:334:GLU:HG3	2.46	0.46
1:A:16:LYS:HG3	1:A:17:ASN:N	2.24	0.46
1:A:16:LYS:C	1:A:18:ILE:H	2.23	0.46
1:A:313:PHE:HA	1:A:320:SER:HA	1.98	0.46
1:A:254:GLU:OE1	1:B:224:SER:HA	2.15	0.46
1:B:345:HIS:CG	1:B:383:MET:HE2	2.51	0.46
1:C:284:ARG:NH2	1:C:322:GLU:O	2.35	0.46
1:D:20:MET:HG3	1:D:23:PHE:CE1	2.51	0.46
1:F:112:SER:HA	1:F:120:VAL:HG21	1.97	0.46
1:F:247:ASN:ND2	2:F:481:HOH:O	2.49	0.45
1:A:288:LYS:HG3	1:A:324:TYR:CZ	2.51	0.45
1:A:307:PRO:HG2	1:A:329:TRP:HB3	1.99	0.45
1:B:382:ASN:O	1:B:386:ILE:HB	2.16	0.45
1:E:217:LLP:OP3	1:F:249:ILE:HD12	2.16	0.45
1:F:387:LYS:HD2	1:F:387:LYS:HA	1.62	0.45
1:B:289:ASN:OD1	1:B:293:LYS:HD2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ILE:HD11	1:D:101:THR:HG21	1.99	0.45
1:C:291:TRP:O	1:C:295:ARG:HB2	2.16	0.45
1:E:334:GLU:OE1	1:E:387:LYS:HG3	2.17	0.45
1:E:338:LEU:HD23	1:E:362:VAL:HG22	1.97	0.45
1:F:225:ARG:HA	1:F:225:ARG:NE	2.31	0.45
1:F:313:PHE:HA	1:F:320:SER:HA	1.98	0.45
1:C:138:TYR:O	1:D:143:MET:HE1	2.17	0.45
1:D:275:GLU:HG2	1:D:281:LYS:HD2	1.99	0.45
1:A:134:GLU:H	1:A:134:GLU:HG2	1.30	0.45
1:A:269:THR:HG23	1:A:279:PHE:H	1.80	0.45
1:B:42:MET:O	1:B:45:ARG:HG2	2.16	0.45
1:C:249:ILE:CG1	1:D:101:THR:HG21	2.47	0.45
1:C:284:ARG:NH2	1:C:321:LEU:HB2	2.32	0.45
1:F:55:LEU:HD13	1:F:253:LYS:HB3	1.99	0.45
1:F:307:PRO:CG	1:F:329:TRP:HB3	2.46	0.45
1:A:309:TYR:CZ	1:A:325:PRO:HG2	2.52	0.45
1:B:169:PRO:HB3	1:B:363:ARG:HD3	1.98	0.45
1:B:142:GLY:HA2	2:B:413:HOH:O	2.16	0.45
1:C:294:LEU:O	1:C:298:VAL:HG23	2.17	0.45
1:C:373:PHE:O	1:C:376:PHE:HB3	2.17	0.45
1:D:19:PRO:CG	1:D:22:ASP:HB2	2.47	0.45
1:A:258:ARG:HD3	1:B:254:GLU:OE2	2.17	0.44
1:D:63:THR:O	1:D:63:THR:CG2	2.65	0.44
1:D:221:HIS:HB3	2:D:400:HOH:O	2.17	0.44
1:E:335:GLU:H	1:E:387:LYS:HA	1.82	0.44
1:E:343:ARG:HB2	1:E:343:ARG:HH11	1.82	0.44
1:F:23:PHE:O	1:F:379:ARG:NH2	2.40	0.44
1:F:232:LYS:NZ	2:F:428:HOH:O	2.50	0.44
1:A:249:ILE:HG13	1:B:101:THR:HG21	2.00	0.44
1:A:344:ARG:NH1	1:A:344:ARG:CB	2.69	0.44
1:A:382:ASN:N	1:A:382:ASN:HD22	2.14	0.44
1:C:134:GLU:H	1:C:134:GLU:HG2	1.49	0.44
1:D:226:ILE:HG21	1:D:259:THR:HG21	1.99	0.44
1:E:138:TYR:O	1:F:109:HIS:HE1	2.00	0.44
1:F:40:ARG:HH11	1:F:40:ARG:HD2	1.57	0.44
1:F:97:GLY:HA2	1:F:251:VAL:HG21	1.98	0.44
1:D:92:ARG:HB2	1:D:231:VAL:O	2.17	0.44
1:E:204:ARG:NH2	2:E:419:HOH:O	2.51	0.44
1:F:55:LEU:HB3	1:F:253:LYS:CB	2.47	0.44
1:F:314:CYS:O	1:F:318:GLY:N	2.50	0.44
1:A:55:LEU:HB3	1:A:253:LYS:CB	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LYS:HB2	1:A:156:LYS:HE2	1.75	0.44
1:D:291:TRP:CD1	1:D:324:TYR:HB3	2.52	0.44
1:E:42:MET:HB3	1:E:46:CYS:SG	2.57	0.44
1:E:297:VAL:CG2	2:E:524:HOH:O	2.48	0.44
1:D:382:ASN:HD22	1:D:382:ASN:HA	1.61	0.44
1:F:145:LYS:HA	2:F:494:HOH:O	2.17	0.44
1:D:322:GLU:HB3	2:D:437:HOH:O	2.17	0.44
1:E:170:ASP:HA	1:E:329:TRP:HB2	1.99	0.44
1:E:52:GLY:HA3	1:F:46:CYS:HB2	2.00	0.44
1:E:269:THR:HG23	1:E:279:PHE:H	1.81	0.44
1:F:262:ILE:HD13	1:F:262:ILE:HG21	1.73	0.44
1:E:201:PRO:HB3	1:E:314:CYS:HB2	2.00	0.43
1:F:18:ILE:HA	2:F:545:HOH:O	2.18	0.43
1:D:73:LEU:O	1:D:77:ILE:HG13	2.17	0.43
1:F:89:THR:HA	1:F:92:ARG:HD2	2.00	0.43
1:A:55:LEU:HB3	1:A:253:LYS:HB3	2.00	0.43
1:D:153:PHE:CE2	1:D:155:LYS:HB2	2.53	0.43
1:B:371:ASP:O	1:B:375:VAL:HG23	2.18	0.43
1:B:384:LYS:HD3	1:B:384:LYS:HA	1.82	0.43
1:C:201:PRO:HA	2:C:396:HOH:O	2.17	0.43
1:C:332:THR:HG21	1:C:336:THR:OG1	2.18	0.43
1:A:27:LEU:HD13	1:A:364:VAL:HG23	2.01	0.43
1:B:63:THR:O	1:B:63:THR:CG2	2.65	0.43
1:B:291:TRP:HH2	2:B:483:HOH:O	2.01	0.43
1:D:272:SER:HB2	2:D:468:HOH:O	2.18	0.43
1:C:328:ALA:HA	2:C:461:HOH:O	2.19	0.43
1:E:369:ARG:NE	2:E:404:HOH:O	2.51	0.43
1:A:170:ASP:HA	1:A:329:TRP:HB2	2.01	0.43
1:B:26:ASN:HA	1:B:348:MET:HB2	2.01	0.43
1:B:291:TRP:O	1:B:295:ARG:HB2	2.18	0.43
1:C:215:PHE:CE1	1:C:221:HIS:HB2	2.54	0.43
1:D:281:LYS:HD3	1:D:281:LYS:O	2.18	0.43
1:E:138:TYR:CE2	1:E:139:VAL:HG13	2.54	0.43
1:A:165:SER:HA	1:A:166:PRO:C	2.44	0.43
1:B:294:LEU:O	1:B:298:VAL:HG23	2.19	0.43
1:C:296:GLU:O	1:C:299:LYS:HB3	2.19	0.43
1:D:165:SER:HA	1:D:166:PRO:C	2.43	0.43
1:F:90:GLU:HB3	2:F:522:HOH:O	2.18	0.43
1:F:281:LYS:HD3	1:F:281:LYS:O	2.19	0.43
1:F:71:PRO:O	1:F:72:GLU:C	2.62	0.43
1:B:268:GLU:O	1:B:271:LYS:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:THR:HG23	1:B:278:ASN:HA	1.99	0.43
1:C:165:SER:HA	1:C:166:PRO:C	2.42	0.43
1:D:36:GLU:HB3	2:D:448:HOH:O	2.19	0.43
1:E:63:THR:O	1:E:63:THR:CG2	2.66	0.43
1:B:350:ARG:HB3	1:B:363:ARG:HB3	2.00	0.42
1:C:156:LYS:O	1:C:156:LYS:HE2	2.19	0.42
1:D:156:LYS:HD2	1:D:156:LYS:N	2.33	0.42
1:B:98:THR:HG23	1:B:102:GLN:OE1	2.19	0.42
1:B:278:ASN:ND2	2:B:407:HOH:O	2.51	0.42
1:E:261:LYS:O	1:E:265:VAL:HG23	2.19	0.42
1:D:247:ASN:ND2	2:D:506:HOH:O	2.51	0.42
1:E:140:ARG:HD3	1:F:143:MET:CG	2.49	0.42
1:F:131:THR:O	1:F:135:GLU:HG3	2.19	0.42
1:F:322:GLU:HB3	2:F:445:HOH:O	2.19	0.42
1:B:321:LEU:N	1:B:321:LEU:CD2	2.82	0.42
1:C:143:MET:CG	1:D:140:ARG:HG3	2.49	0.42
1:C:198:HIS:HA	1:C:284:ARG:HB2	2.01	0.42
1:C:382:ASN:HD22	1:C:382:ASN:N	2.17	0.42
1:A:61:ASP:CG	1:A:63:THR:HB	2.43	0.42
1:A:341:GLU:O	1:A:344:ARG:HB2	2.19	0.42
1:B:215:PHE:HZ	1:B:262:ILE:HG12	1.84	0.42
1:C:65:LEU:HD21	1:C:238:LYS:N	2.35	0.42
1:F:274:SER:HB3	1:F:277:GLU:CB	2.31	0.42
1:B:69:LEU:HD13	1:B:96:VAL:HB	2.02	0.42
1:C:101:THR:HG21	1:D:249:ILE:HG13	2.02	0.42
1:C:200:THR:OG1	1:C:201:PRO:HD2	2.20	0.42
1:F:383:MET:HE3	1:F:383:MET:HB2	1.89	0.42
1:C:298:VAL:HG13	1:C:304:PHE:HB2	2.02	0.42
1:D:215:PHE:CE1	1:D:221:HIS:HB2	2.55	0.42
1:F:259:THR:O	1:F:263:LEU:HG	2.18	0.42
1:A:334:GLU:H	1:A:334:GLU:HG2	1.56	0.42
1:B:21:SER:O	1:B:346:LYS:HD2	2.20	0.42
1:C:25:VAL:HG12	1:C:27:LEU:HG	2.01	0.42
1:D:161:GLU:OE2	1:D:177:VAL:HG22	2.20	0.42
1:D:241:VAL:O	1:D:245:ILE:HG13	2.19	0.42
1:E:371:ASP:O	1:E:375:VAL:HG23	2.20	0.42
1:F:20:MET:O	1:F:21:SER:HB3	2.13	0.42
1:F:371:ASP:OD1	1:F:371:ASP:N	2.52	0.42
1:B:90:GLU:OE2	1:B:205:ARG:NH2	2.52	0.42
1:B:345:HIS:CD2	2:B:574:HOH:O	2.73	0.42
1:C:18:ILE:O	1:C:20:MET:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:GLU:OE2	1:D:205:ARG:NH2	2.53	0.42
1:E:55:LEU:HD11	1:E:257:VAL:HG21	2.02	0.42
1:E:61:ASP:OD1	1:E:63:THR:HB	2.19	0.42
1:B:375:VAL:HG12	1:B:379:ARG:HD2	2.02	0.42
1:D:125:ALA:O	1:D:174:ARG:NH1	2.47	0.42
1:E:376:PHE:O	1:E:380:LEU:HB2	2.20	0.42
1:A:262:ILE:HD12	1:A:262:ILE:HG23	1.67	0.41
1:B:234:LYS:HE2	1:B:234:LYS:HB3	1.80	0.41
1:E:303:ALA:HB1	1:E:334:GLU:HG3	2.02	0.41
1:B:156:LYS:H	1:B:156:LYS:CD	2.17	0.41
1:C:342:LEU:HD12	1:C:383:MET:HE1	2.02	0.41
1:D:55:LEU:HB3	1:D:253:LYS:CB	2.50	0.41
1:A:304:PHE:HZ	1:A:383:MET:HE2	1.86	0.41
1:D:170:ASP:HA	1:D:329:TRP:HB2	2.03	0.41
1:F:80:LEU:HD13	1:F:196:TRP:CH2	2.56	0.41
1:C:254:GLU:OE2	1:D:258:ARG:HD3	2.20	0.41
1:C:343:ARG:HG3	1:C:348:MET:CE	2.48	0.41
1:D:343:ARG:HG3	1:D:348:MET:CE	2.50	0.41
1:F:167:ASN:HB2	1:F:174:ARG:HD2	2.02	0.41
1:F:339:VAL:HG21	1:F:351:ALA:HB2	2.02	0.41
1:B:101:THR:HB	2:B:398:HOH:O	2.20	0.41
1:B:225:ARG:NE	1:B:225:ARG:CA	2.82	0.41
1:D:42:MET:O	1:D:45:ARG:HG3	2.20	0.41
1:C:314:CYS:O	1:C:318:GLY:N	2.52	0.41
1:A:129:TYR:CE2	1:A:131:THR:HB	2.55	0.41
1:E:328:ALA:O	1:E:364:VAL:HG12	2.21	0.41
1:B:328:ALA:HB3	1:B:364:VAL:CG1	2.44	0.41
1:F:72:GLU:CD	1:F:72:GLU:H	2.29	0.41
1:F:344:ARG:NH1	1:F:344:ARG:CG	2.83	0.41
1:A:129:TYR:CZ	1:A:131:THR:HB	2.55	0.41
1:A:321:LEU:H	1:A:321:LEU:HD23	1.86	0.41
1:B:70:GLU:HA	1:B:71:PRO:HD3	1.96	0.41
1:B:383:MET:C	1:B:385:LEU:N	2.79	0.41
1:C:55:LEU:HB3	1:C:253:LYS:CG	2.51	0.41
1:C:214:THR:OG1	1:C:217:LLP:OP1	2.37	0.41
1:D:343:ARG:HG3	1:D:348:MET:HE1	2.01	0.41
1:E:63:THR:O	1:E:63:THR:HG22	2.21	0.41
1:F:97:GLY:HA2	1:F:251:VAL:CG2	2.51	0.41
1:A:111:LEU:HD22	1:A:187:LYS:HG3	2.02	0.41
1:A:282:TYR:CD1	1:A:282:TYR:C	2.99	0.40
1:C:224:SER:HA	1:D:254:GLU:OE1	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:LEU:O	1:D:342:LEU:HB2	2.22	0.40
1:A:80:LEU:HD12	1:A:196:TRP:CH2	2.56	0.40
1:A:129:TYR:HB3	1:A:132:TYR:CD2	2.57	0.40
1:E:233:ASP:OD2	1:E:236:VAL:HG23	2.20	0.40
1:B:161:GLU:OE1	1:B:178:VAL:CG1	2.66	0.40
1:B:345:HIS:HD2	2:B:574:HOH:O	2.04	0.40
1:C:103:LEU:HB3	1:C:212:LEU:HD22	2.02	0.40
1:E:125:ALA:O	1:E:174:ARG:NH1	2.53	0.40
1:C:111:LEU:HD13	1:C:187:LYS:CB	2.51	0.40
1:C:284:ARG:HH21	1:C:321:LEU:HB2	1.86	0.40
1:E:201:PRO:CB	1:E:314:CYS:HB2	2.52	0.40
1:F:63:THR:O	1:F:63:THR:HG23	2.20	0.40
1:F:188:VAL:HG11	1:F:190:HIS:CE1	2.55	0.40
1:F:252:SER:O	1:F:256:GLN:HG3	2.21	0.40
1:F:266:LEU:HD23	1:F:266:LEU:O	2.21	0.40
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.88	0.40
1:B:84:VAL:HA	1:B:316:TYR:CD1	2.57	0.40
1:B:204:ARG:HB3	2:B:408:HOH:O	2.22	0.40
1:D:55:LEU:HD13	1:D:253:LYS:HB3	2.03	0.40
1:D:129:TYR:CE2	1:D:131:THR:HB	2.57	0.40
1:D:129:TYR:HB3	1:D:132:TYR:CD2	2.56	0.40
1:E:303:ALA:HB2	1:E:334:GLU:OE2	2.21	0.40
1:F:25:VAL:HG12	1:F:27:LEU:HG	2.03	0.40
1:F:226:ILE:HG21	1:F:259:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	358/391 (92%)	337 (94%)	20 (6%)	1 (0%)	36 50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	359/391 (92%)	334 (93%)	20 (6%)	5 (1%)	9	13
1	C	355/391 (91%)	330 (93%)	23 (6%)	2 (1%)	21	32
1	D	355/391 (91%)	332 (94%)	21 (6%)	2 (1%)	21	32
1	E	356/391 (91%)	333 (94%)	21 (6%)	2 (1%)	21	32
1	F	358/391 (92%)	332 (93%)	23 (6%)	3 (1%)	16	25
All	All	2141/2346 (91%)	1998 (93%)	128 (6%)	15 (1%)	18	28

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	386	ILE
1	D	20	MET
1	E	386	ILE
1	F	19	PRO
1	B	248	SER
1	D	19	PRO
1	F	98	THR
1	E	248	SER
1	A	334	GLU
1	B	151	TRP
1	B	382	ASN
1	C	20	MET
1	F	248	SER
1	B	98	THR
1	C	151	TRP

5.3.2 Protein sidechains [i](#)

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	317/345 (92%)	291 (92%)	26 (8%)	10	18
1	B	318/345 (92%)	290 (91%)	28 (9%)	9	15
1	C	314/345 (91%)	286 (91%)	28 (9%)	9	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	314/345 (91%)	286 (91%)	28 (9%)	9	15
1	E	315/345 (91%)	299 (95%)	16 (5%)	21	37
1	F	317/345 (92%)	296 (93%)	21 (7%)	15	26
All	All	1895/2070 (92%)	1748 (92%)	147 (8%)	11	20

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	18	ILE
1	A	20	MET
1	A	37	GLU
1	A	80	LEU
1	A	101	THR
1	A	103	LEU
1	A	113	SER
1	A	134	GLU
1	A	156	LYS
1	A	175	GLU
1	A	214	THR
1	A	254	GLU
1	A	255	SER
1	A	257	VAL
1	A	269	THR
1	A	271	LYS
1	A	295	ARG
1	A	302	ASP
1	A	321	LEU
1	A	334	GLU
1	A	342	LEU
1	A	348	MET
1	A	364	VAL
1	A	369	ARG
1	A	380	LEU
1	B	51	ARG
1	B	63	THR
1	B	72	GLU
1	B	80	LEU
1	B	101	THR
1	B	103	LEU
1	B	134	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	156	LYS
1	B	212	LEU
1	B	225	ARG
1	B	254	GLU
1	B	255	SER
1	B	262	ILE
1	B	269	THR
1	B	275	GLU
1	B	287	MET
1	B	295	ARG
1	B	302	ASP
1	B	306	LEU
1	B	321	LEU
1	B	333	LYS
1	B	342	LEU
1	B	344	ARG
1	B	364	VAL
1	B	378	GLU
1	B	380	LEU
1	B	382	ASN
1	B	386	ILE
1	C	21	SER
1	C	37	GLU
1	C	80	LEU
1	C	101	THR
1	C	103	LEU
1	C	116	ARG
1	C	134	GLU
1	C	156	LYS
1	C	175	GLU
1	C	253	LYS
1	C	254	GLU
1	C	255	SER
1	C	269	THR
1	C	273	GLU
1	C	277	GLU
1	C	295	ARG
1	C	300	GLU
1	C	321	LEU
1	C	334	GLU
1	C	335	GLU
1	C	336	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	342	LEU
1	C	343	ARG
1	C	344	ARG
1	C	364	VAL
1	C	369	ARG
1	C	380	LEU
1	C	384	LYS
1	D	37	GLU
1	D	45	ARG
1	D	51	ARG
1	D	63	THR
1	D	80	LEU
1	D	98	THR
1	D	101	THR
1	D	103	LEU
1	D	134	GLU
1	D	156	LYS
1	D	214	THR
1	D	225	ARG
1	D	231	VAL
1	D	254	GLU
1	D	255	SER
1	D	262	ILE
1	D	267	LYS
1	D	269	THR
1	D	273	GLU
1	D	295	ARG
1	D	302	ASP
1	D	306	LEU
1	D	321	LEU
1	D	342	LEU
1	D	344	ARG
1	D	353	GLU
1	D	364	VAL
1	D	380	LEU
1	E	80	LEU
1	E	101	THR
1	E	103	LEU
1	E	134	GLU
1	E	156	LYS
1	E	254	GLU
1	E	267	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	269	THR
1	E	275	GLU
1	E	295	ARG
1	E	321	LEU
1	E	342	LEU
1	E	343	ARG
1	E	370	GLU
1	E	380	LEU
1	E	382	ASN
1	F	20	MET
1	F	37	GLU
1	F	40	ARG
1	F	63	THR
1	F	80	LEU
1	F	101	THR
1	F	103	LEU
1	F	134	GLU
1	F	176	THR
1	F	187	LYS
1	F	225	ARG
1	F	255	SER
1	F	269	THR
1	F	295	ARG
1	F	306	LEU
1	F	321	LEU
1	F	342	LEU
1	F	364	VAL
1	F	370	GLU
1	F	380	LEU
1	F	387	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	382	ASN
1	B	190	HIS
1	B	208	HIS
1	C	26	ASN
1	C	109	HIS
1	C	264	ASN
1	C	382	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	315	ASN
1	D	382	ASN
1	E	64	ASN
1	E	289	ASN
1	F	109	HIS
1	F	289	ASN
1	F	382	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	A	217	1	23,24,25	2.22	7 (30%)	25,32,34	1.82	6 (24%)
1	LLP	D	217	1	23,24,25	2.23	5 (21%)	25,32,34	1.61	6 (24%)
1	LLP	E	217	1	23,24,25	2.23	7 (30%)	25,32,34	1.48	5 (20%)
1	LLP	F	217	1	23,24,25	2.05	6 (26%)	25,32,34	1.75	5 (20%)
1	LLP	C	217	1	23,24,25	2.06	6 (26%)	25,32,34	1.47	6 (24%)
1	LLP	B	217	1	23,24,25	2.12	5 (21%)	25,32,34	1.46	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	217	1	-	3/16/17/19	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	D	217	1	-	3/16/17/19	0/1/1/1
1	LLP	E	217	1	-	3/16/17/19	0/1/1/1
1	LLP	F	217	1	-	3/16/17/19	0/1/1/1
1	LLP	C	217	1	-	3/16/17/19	0/1/1/1
1	LLP	B	217	1	-	3/16/17/19	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	217	LLP	C4'-NZ	6.26	1.48	1.27
1	A	217	LLP	C4'-NZ	6.14	1.47	1.27
1	F	217	LLP	C4'-NZ	6.11	1.47	1.27
1	B	217	LLP	C4'-NZ	6.04	1.47	1.27
1	C	217	LLP	C4'-NZ	5.91	1.46	1.27
1	E	217	LLP	C4'-NZ	5.75	1.46	1.27
1	D	217	LLP	C6-C5	5.32	1.48	1.37
1	E	217	LLP	C6-C5	5.07	1.47	1.37
1	A	217	LLP	C6-C5	4.60	1.46	1.37
1	B	217	LLP	C6-C5	4.59	1.46	1.37
1	C	217	LLP	C6-C5	4.58	1.46	1.37
1	F	217	LLP	C6-C5	3.71	1.45	1.37
1	E	217	LLP	C4-C4'	3.58	1.54	1.46
1	D	217	LLP	C4-C5	3.58	1.46	1.42
1	B	217	LLP	C4-C5	3.51	1.46	1.42
1	E	217	LLP	C4-C5	3.51	1.46	1.42
1	B	217	LLP	C4-C4'	3.48	1.54	1.46
1	F	217	LLP	C4-C4'	3.35	1.53	1.46
1	F	217	LLP	C4-C5	3.24	1.46	1.42
1	D	217	LLP	C4-C4'	3.13	1.53	1.46
1	A	217	LLP	C4-C4'	3.08	1.53	1.46
1	D	217	LLP	C2-N1	3.01	1.39	1.33
1	C	217	LLP	C4-C4'	2.99	1.53	1.46
1	A	217	LLP	C3-C2	2.93	1.44	1.41
1	A	217	LLP	C2-N1	2.90	1.39	1.33
1	A	217	LLP	C4-C5	2.89	1.46	1.42
1	C	217	LLP	C3-C2	2.87	1.43	1.41
1	E	217	LLP	C3-C2	2.59	1.43	1.41
1	E	217	LLP	P-OP2	-2.53	1.45	1.54
1	E	217	LLP	C2-N1	2.52	1.38	1.33
1	F	217	LLP	P-OP2	-2.50	1.45	1.54
1	C	217	LLP	C4-C5	2.42	1.45	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	LLP	C2-N1	2.41	1.38	1.33
1	A	217	LLP	P-OP2	-2.36	1.46	1.54
1	F	217	LLP	C2-N1	2.06	1.37	1.33
1	C	217	LLP	P-OP2	-2.02	1.47	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	217	LLP	C4-C4'-NZ	-4.05	105.37	124.04
1	A	217	LLP	C5-C6-N1	-3.91	117.47	123.83
1	B	217	LLP	OP4-P-OP1	3.49	115.87	106.44
1	F	217	LLP	OP4-P-OP1	3.46	115.80	106.44
1	D	217	LLP	C5-C6-N1	-3.44	118.23	123.83
1	F	217	LLP	C6-N1-C2	3.41	125.38	119.20
1	D	217	LLP	OP4-P-OP1	3.40	115.62	106.44
1	E	217	LLP	C4-C4'-NZ	-3.30	108.81	124.04
1	C	217	LLP	C4-C4'-NZ	-3.21	109.25	124.04
1	B	217	LLP	C4-C4'-NZ	-3.19	109.32	124.04
1	A	217	LLP	OP4-P-OP1	3.17	115.02	106.44
1	A	217	LLP	C4-C4'-NZ	-3.16	109.45	124.04
1	A	217	LLP	O3-C3-C2	3.06	123.92	117.58
1	C	217	LLP	C5-C6-N1	-3.00	118.96	123.83
1	C	217	LLP	OP4-P-OP1	2.95	114.41	106.44
1	F	217	LLP	C5-C6-N1	-2.94	119.05	123.83
1	B	217	LLP	C5-C6-N1	-2.87	119.16	123.83
1	E	217	LLP	CE-NZ-C4'	2.86	127.86	118.72
1	E	217	LLP	C5-C6-N1	-2.85	119.20	123.83
1	D	217	LLP	C4-C4'-NZ	-2.81	111.09	124.04
1	A	217	LLP	C6-N1-C2	2.73	124.15	119.20
1	D	217	LLP	C5'-C5-C6	2.70	123.76	119.36
1	B	217	LLP	CE-NZ-C4'	2.55	126.89	118.72
1	E	217	LLP	OP4-C5'-C5	2.44	113.92	109.36
1	F	217	LLP	CE-NZ-C4'	2.37	126.31	118.72
1	A	217	LLP	CE-NZ-C4'	2.29	126.06	118.72
1	D	217	LLP	C6-N1-C2	2.27	123.31	119.20
1	C	217	LLP	CE-NZ-C4'	2.26	125.95	118.72
1	C	217	LLP	C6-N1-C2	2.23	123.25	119.20
1	D	217	LLP	CE-NZ-C4'	2.15	125.61	118.72
1	B	217	LLP	C5'-C5-C6	2.14	122.85	119.36
1	E	217	LLP	OP4-P-OP1	2.14	112.23	106.44
1	C	217	LLP	OP4-C5'-C5	2.05	113.19	109.36

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	217	LLP	C3-C4-C4'-NZ
1	C	217	LLP	CG-CD-CE-NZ
1	E	217	LLP	CG-CD-CE-NZ
1	C	217	LLP	C3-C4-C4'-NZ
1	D	217	LLP	C3-C4-C4'-NZ
1	A	217	LLP	CG-CD-CE-NZ
1	B	217	LLP	CG-CD-CE-NZ
1	D	217	LLP	CG-CD-CE-NZ
1	F	217	LLP	CG-CD-CE-NZ
1	A	217	LLP	C3-C4-C4'-NZ
1	B	217	LLP	C3-C4-C4'-NZ
1	E	217	LLP	C3-C4-C4'-NZ
1	A	217	LLP	C5-C4-C4'-NZ
1	D	217	LLP	C5-C4-C4'-NZ
1	B	217	LLP	C5-C4-C4'-NZ
1	C	217	LLP	C5-C4-C4'-NZ
1	E	217	LLP	C5-C4-C4'-NZ
1	F	217	LLP	CD-CE-NZ-C4'

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	217	LLP	2	0
1	D	217	LLP	3	0
1	E	217	LLP	3	0
1	F	217	LLP	3	0
1	C	217	LLP	3	0
1	B	217	LLP	3	0

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	362/391 (92%)	-1.72	0 100 100	8, 30, 60, 74	0
1	B	363/391 (92%)	-1.68	0 100 100	8, 29, 61, 74	0
1	C	359/391 (91%)	-1.66	0 100 100	14, 32, 61, 77	0
1	D	359/391 (91%)	-1.69	0 100 100	11, 31, 61, 77	0
1	E	360/391 (92%)	-1.66	0 100 100	14, 32, 58, 71	0
1	F	362/391 (92%)	-1.69	0 100 100	12, 30, 59, 77	0
All	All	2165/2346 (92%)	-1.68	0 100 100	8, 31, 61, 77	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	A	217	24/25	1.00	0.02	18,23,25,29	0
1	LLP	B	217	24/25	1.00	0.02	18,21,25,29	0
1	LLP	C	217	24/25	1.00	0.02	23,25,29,32	0
1	LLP	D	217	24/25	1.00	0.02	19,23,32,37	0
1	LLP	E	217	24/25	1.00	0.02	18,23,26,27	0
1	LLP	F	217	24/25	1.00	0.02	15,23,27,32	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.