



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 PM GMT

PDB ID : 4LLF
Title : Crystal structure of Cucumber Necrosis Virus
Authors : Smith, T.
Deposited on : 2013-07-09
Resolution : 2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

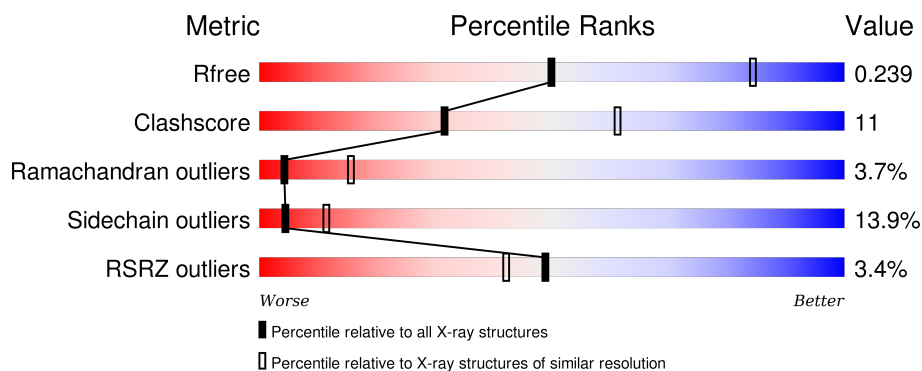
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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

Mol	Chain	Length	Quality of chain
1	A	380	<div> <div>2%</div> <div>52% 20% 24%</div> </div>
1	B	380	<div> <div>4%</div> <div>50% 20% 5% 23%</div> </div>
1	D	380	<div> <div>%</div> <div>56% 25% 16%</div> </div>
1	E	380	<div> <div>%</div> <div>52% 21% 24%</div> </div>
1	F	380	<div> <div>3%</div> <div>49% 21% 6% 23%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	380	
1	H	380	
1	I	380	
1	J	380	
1	K	380	
1	L	380	
1	M	380	
1	N	380	
1	O	380	
1	P	380	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	B	401	-	-	-	X
2	CA	E	402	-	-	-	X
2	CA	K	402	-	-	-	X
2	CA	N	401	-	-	-	X
2	CA	O	402	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34586 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	1	0
			2212	1408	370	433	1			
1	B	291	Total	C	N	O	S	0	1	0
			2226	1417	373	435	1			
1	D	321	Total	C	N	O	S	0	2	0
			2462	1573	417	471	1			
1	E	289	Total	C	N	O	S	0	1	0
			2212	1408	370	433	1			
1	F	291	Total	C	N	O	S	0	1	0
			2226	1417	373	435	1			
1	G	321	Total	C	N	O	S	0	2	0
			2462	1573	417	471	1			
1	H	289	Total	C	N	O	S	0	1	0
			2212	1408	370	433	1			
1	I	291	Total	C	N	O	S	0	1	0
			2226	1417	373	435	1			
1	J	321	Total	C	N	O	S	0	2	0
			2462	1573	417	471	1			
1	K	289	Total	C	N	O	S	0	1	0
			2212	1408	370	433	1			
1	L	291	Total	C	N	O	S	0	1	0
			2226	1417	373	435	1			
1	M	321	Total	C	N	O	S	0	2	0
			2462	1573	417	471	1			
1	N	289	Total	C	N	O	S	0	1	0
			2212	1408	370	433	1			
1	O	291	Total	C	N	O	S	0	1	0
			2226	1417	373	435	1			
1	P	321	Total	C	N	O	S	0	2	0
			2462	1573	417	471	1			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Ca 1 1	0	0
2	K	2	Total Ca 2 2	0	0
2	E	2	Total Ca 2 2	0	0
2	H	1	Total Ca 1 1	0	0
2	B	2	Total Ca 2 2	0	0
2	I	2	Total Ca 2 2	0	0
2	N	1	Total Ca 1 1	0	0
2	O	2	Total Ca 2 2	0	0
2	F	1	Total Ca 1 1	0	0
2	M	1	Total Ca 1 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Zn 2 2	0	1
3	G	1	Total Zn 2 2	0	1
3	J	1	Total Zn 2 2	0	1
3	D	1	Total Zn 2 2	0	1
3	M	1	Total Zn 2 2	0	1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	5	Total O 5 5	0	0
4	D	4	Total O 4 4	0	0

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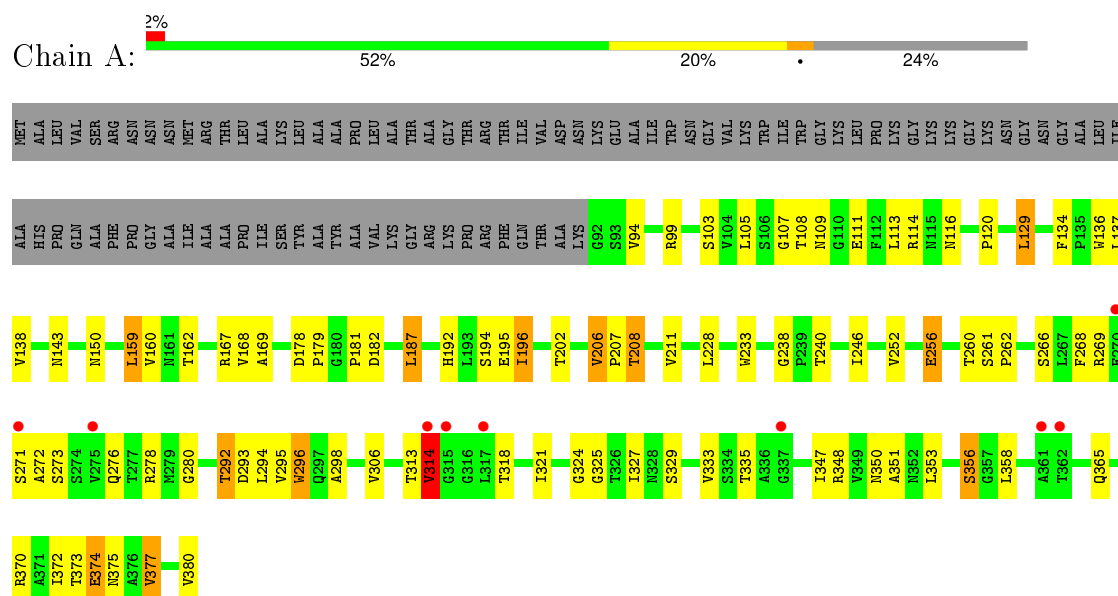
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	3	Total 3	O 3	0	0
4	F	1	Total 1	O 1	0	0
4	G	5	Total 5	O 5	0	0
4	H	4	Total 4	O 4	0	0
4	I	3	Total 3	O 3	0	0
4	J	3	Total 3	O 3	0	0
4	K	3	Total 3	O 3	0	0
4	L	5	Total 5	O 5	0	0
4	M	4	Total 4	O 4	0	0
4	N	5	Total 5	O 5	0	0
4	O	4	Total 4	O 4	0	0
4	P	7	Total 7	O 7	0	0

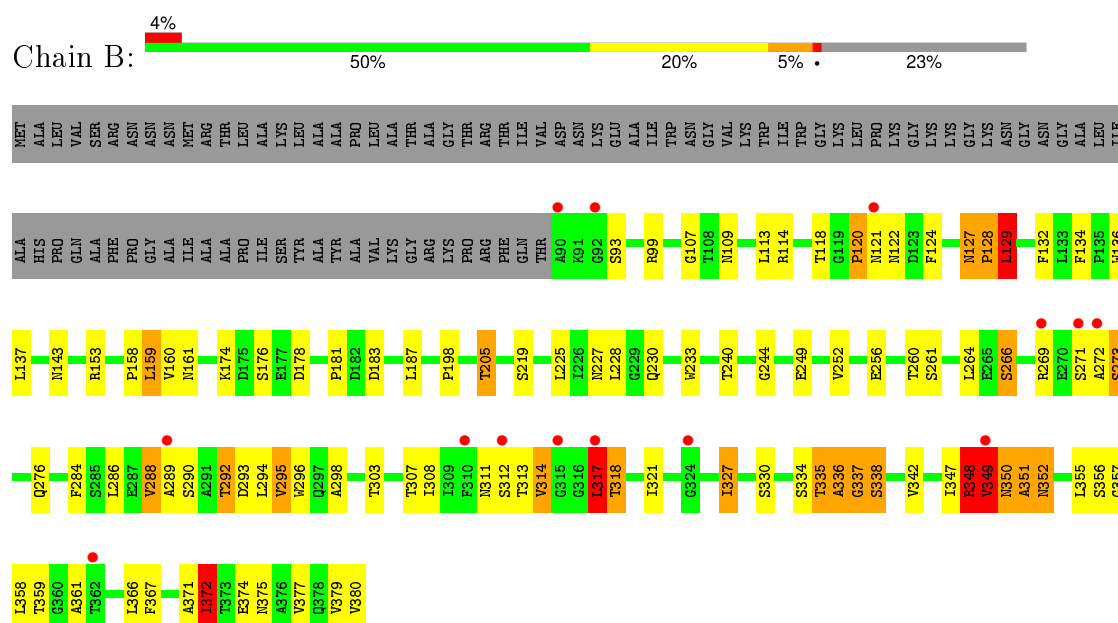
3 Residue-property plots

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

• Molecule 1: Capsid protein

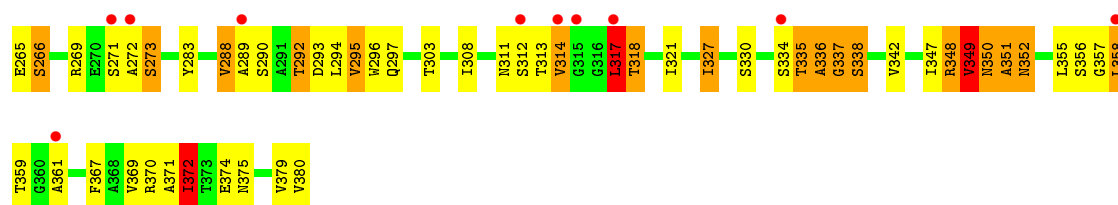


• Molecule 1: Capsid protein

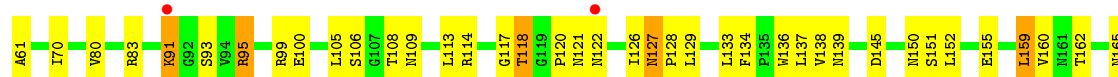


Chain D: 56% 25% 16%

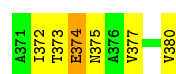
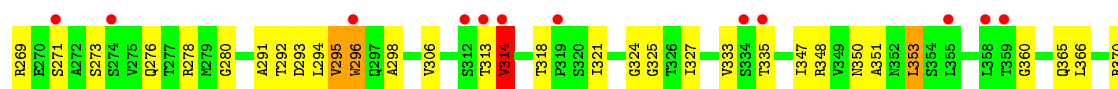
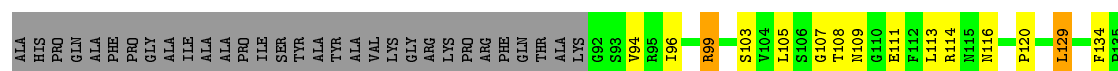




• Molecule 1: Capsid protein

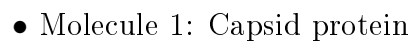


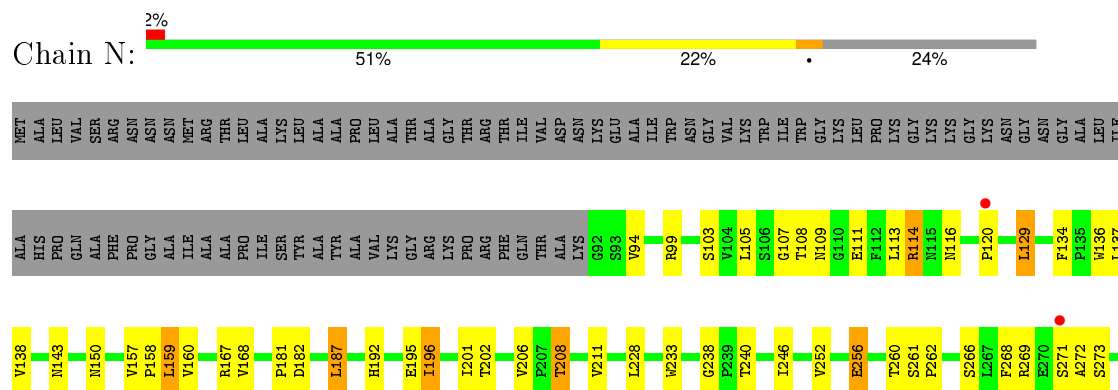
• Molecule 1: Capsid protein

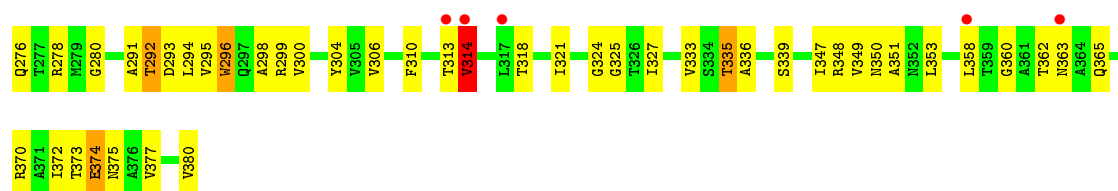


• Molecule 1: Capsid protein

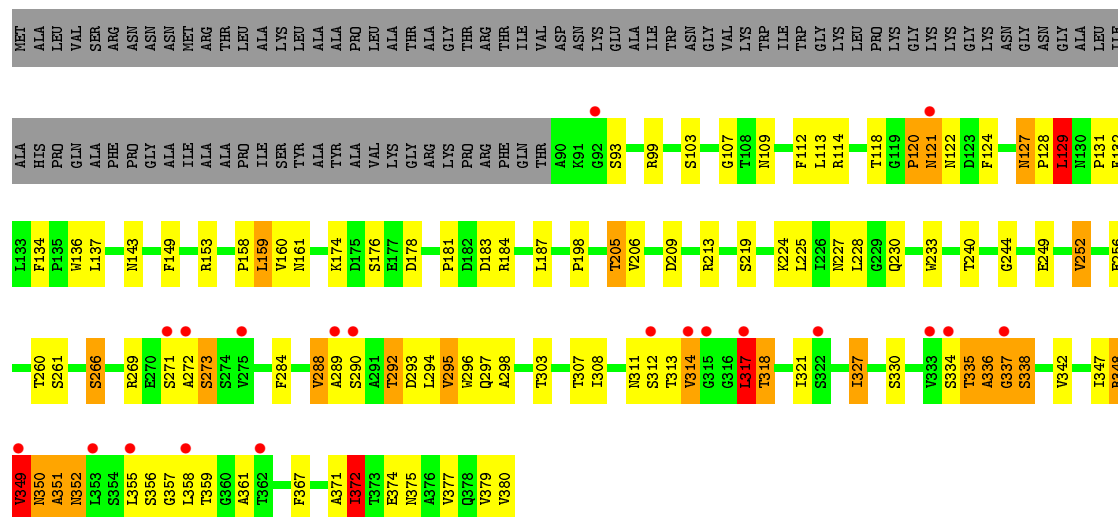




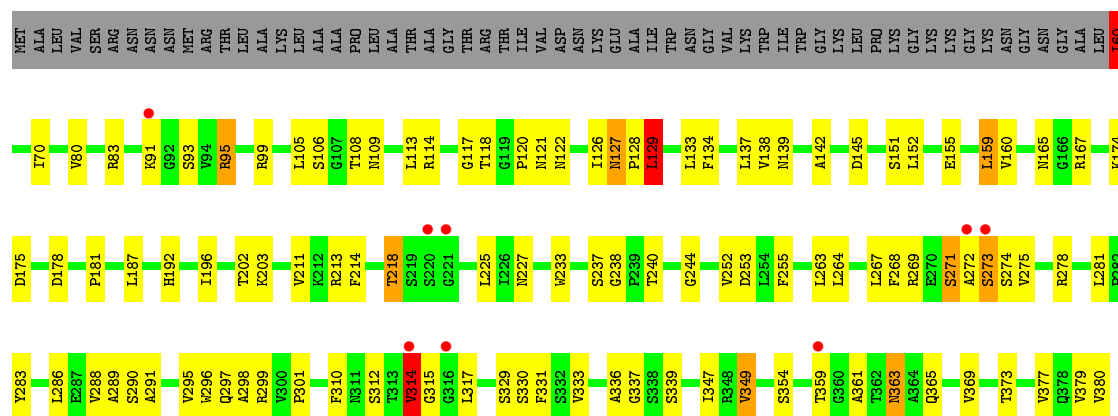




• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	384.00Å 384.00Å 384.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.31 – 2.89 78.38 – 2.89	Depositor EDS
% Data completeness (in resolution range)	64.4 (75.31-2.89) 63.6 (78.38-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.213 , 0.242 0.205 , 0.239	Depositor DCC
R_{free} test set	6788 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.3	EDS
Estimated twinning fraction	0.013 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 191574 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	34586	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.54	0/2267	0.67	1/3102 (0.0%)
1	B	0.54	0/2281	0.74	5/3120 (0.2%)
1	D	0.53	0/2530	0.74	4/3461 (0.1%)
1	E	0.55	0/2267	0.66	0/3102
1	F	0.56	2/2281 (0.1%)	0.72	4/3120 (0.1%)
1	G	0.53	0/2530	0.76	2/3461 (0.1%)
1	H	0.76	7/2267 (0.3%)	0.80	6/3102 (0.2%)
1	I	0.55	0/2281	0.83	10/3120 (0.3%)
1	J	0.54	0/2530	0.77	4/3461 (0.1%)
1	K	0.54	0/2267	0.67	0/3102
1	L	0.53	0/2281	0.71	3/3120 (0.1%)
1	M	0.53	0/2530	0.77	6/3461 (0.2%)
1	N	0.52	0/2267	0.67	0/3102
1	O	0.53	2/2281 (0.1%)	0.70	3/3120 (0.1%)
1	P	0.52	0/2530	0.74	4/3461 (0.1%)
All	All	0.55	11/35390 (0.0%)	0.73	52/48415 (0.1%)

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	L	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	296	TRP	CG-CD1	-18.62	1.10	1.36
1	H	296	TRP	CE3-CZ3	7.97	1.52	1.38
1	H	296	TRP	CZ3-CH2	-7.36	1.28	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	296	TRP	CD2-CE3	-7.21	1.29	1.40
1	H	296	TRP	CB-CG	-6.82	1.38	1.50
1	H	296	TRP	NE1-CE2	-6.68	1.28	1.37
1	H	296	TRP	CD1-NE1	-6.21	1.27	1.38
1	F	297	GLN	CD-NE2	-5.70	1.18	1.32
1	O	297	GLN	CD-NE2	-5.56	1.19	1.32
1	F	297	GLN	CD-OE1	-5.29	1.12	1.24
1	O	297	GLN	CD-OE1	-5.15	1.12	1.24

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	348	ARG	NE-CZ-NH1	-14.80	112.90	120.30
1	I	348	ARG	NE-CZ-NH2	14.07	127.33	120.30
1	H	296	TRP	CG-CD1-NE1	12.98	123.08	110.10
1	H	296	TRP	CB-CG-CD2	11.38	141.39	126.60
1	M	60	ILE	CG1-CB-CG2	-10.28	88.78	111.40
1	H	296	TRP	CB-CG-CD1	-9.72	114.36	127.00
1	J	60	ILE	CG1-CB-CG2	-9.48	90.55	111.40
1	B	348	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	G	60	ILE	CG1-CB-CG2	-8.10	93.57	111.40
1	L	127	ASN	C-N-CD	-8.04	102.91	120.60
1	P	60	ILE	CG1-CB-CG2	-8.00	93.81	111.40
1	D	60	ILE	CG1-CB-CG2	-7.82	94.21	111.40
1	H	296	TRP	CE2-CD2-CG	-6.92	101.76	107.30
1	J	210	ASN	CB-CA-C	6.83	124.05	110.40
1	D	127	ASN	C-N-CA	-6.51	94.66	122.00
1	P	127	ASN	C-N-CA	-6.42	95.02	122.00
1	O	317	LEU	CA-CB-CG	6.38	129.97	115.30
1	I	330	SER	CB-CA-C	6.34	122.15	110.10
1	M	127	ASN	C-N-CA	-6.28	95.64	122.00
1	H	296	TRP	CD1-CG-CD2	-6.19	101.35	106.30
1	L	317	LEU	CA-CB-CG	6.19	129.53	115.30
1	J	127	ASN	C-N-CA	-6.14	96.22	122.00
1	A	356	SER	N-CA-CB	-6.11	101.34	110.50
1	G	127	ASN	C-N-CA	-6.05	96.60	122.00
1	B	317	LEU	CA-CB-CG	6.00	129.10	115.30
1	L	129	LEU	N-CA-C	6.00	127.19	111.00
1	F	317	LEU	CA-CB-CG	5.88	128.82	115.30
1	I	330	SER	CA-CB-OG	5.86	127.02	111.20
1	F	127	ASN	C-N-CA	-5.85	97.44	122.00
1	I	127	ASN	C-N-CA	-5.84	97.49	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	317	LEU	CA-CB-CG	5.83	128.71	115.30
1	O	127	ASN	C-N-CA	-5.77	97.76	122.00
1	I	348	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	127	ASN	C-N-CA	-5.61	98.42	122.00
1	D	83	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	129	LEU	N-CA-C	5.45	125.72	111.00
1	I	129	LEU	N-CA-C	5.37	125.49	111.00
1	F	129	LEU	N-CA-C	5.35	125.45	111.00
1	J	314	VAL	CB-CA-C	5.26	121.39	111.40
1	P	314	VAL	CB-CA-C	5.26	121.39	111.40
1	I	128	PRO	C-N-CA	5.20	134.70	121.70
1	P	129	LEU	N-CA-C	5.20	125.04	111.00
1	O	129	LEU	N-CA-C	5.20	125.04	111.00
1	F	128	PRO	C-N-CA	5.19	134.67	121.70
1	M	129	LEU	N-CA-C	5.17	124.96	111.00
1	I	252	VAL	CB-CA-C	-5.16	101.59	111.40
1	M	314	VAL	CB-CA-C	5.15	121.18	111.40
1	D	129	LEU	N-CA-C	5.09	124.73	111.00
1	M	99[A]	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	M	99[B]	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	H	296	TRP	CA-CB-CG	-5.04	104.12	113.70
1	B	128	PRO	C-N-CA	5.03	134.28	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	128	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	2212	0	2159	45	0
1	B	2226	0	2177	54	0
1	D	2462	0	2418	49	0
1	E	2212	0	2159	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2226	0	2177	56	0
1	G	2462	0	2418	49	0
1	H	2212	0	2159	57	0
1	I	2226	0	2177	59	0
1	J	2462	0	2418	51	0
1	K	2212	0	2159	44	0
1	L	2226	0	2177	62	0
1	M	2462	0	2418	50	0
1	N	2212	0	2159	50	0
1	O	2226	0	2177	58	0
1	P	2462	0	2418	49	0
2	B	2	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
2	I	2	0	0	0	0
2	K	2	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	2	0	0	0	0
3	D	2	0	0	0	0
3	G	2	0	0	0	0
3	J	2	0	0	0	0
3	M	2	0	0	0	0
3	P	2	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	1	0	0	0	0
4	G	5	0	0	0	0
4	H	4	0	0	1	0
4	I	3	0	0	1	0
4	J	3	0	0	0	0
4	K	3	0	0	0	0
4	L	5	0	0	2	0
4	M	4	0	0	0	0
4	N	5	0	0	1	0
4	O	4	0	0	0	0
4	P	7	0	0	0	0
All	All	34586	0	33770	727	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 11.

All (727) 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:H:296:TRP:CZ3	1:H:366:LEU:HB2	1.73	1.24
1:H:296:TRP:HE3	1:H:366:LEU:HD22	1.19	1.07
1:H:296:TRP:HZ3	1:H:366:LEU:HB2	1.20	1.01
1:H:296:TRP:HD1	1:H:296:TRP:N	1.56	0.98
1:J:122:ASN:HB3	1:J:218:THR:HG21	1.56	0.87
1:H:295:VAL:C	1:H:296:TRP:HD1	1.78	0.87
1:H:296:TRP:CE3	1:H:366:LEU:HD22	2.10	0.86
1:H:296:TRP:CE3	1:H:366:LEU:HB2	2.10	0.86
1:L:348:ARG:HG2	1:L:349:VAL:HG12	1.64	0.79
1:J:109:ASN:H	1:J:240:THR:HB	1.48	0.79
1:H:296:TRP:CD1	1:H:296:TRP:N	2.41	0.78
1:L:335:THR:OG1	1:L:336:ALA:N	2.18	0.77
1:F:335:THR:OG1	1:F:336:ALA:N	2.18	0.77
1:O:335:THR:OG1	1:O:336:ALA:N	2.18	0.76
1:F:348:ARG:HG2	1:F:349:VAL:HG12	1.67	0.74
1:I:335:THR:OG1	1:I:336:ALA:N	2.19	0.74
1:F:109:ASN:H	1:F:240:THR:HB	1.54	0.73
1:L:128:PRO:O	1:L:141:ALA:CB	2.37	0.73
1:M:109:ASN:H	1:M:240:THR:HB	1.54	0.73
1:G:109:ASN:H	1:G:240:THR:HB	1.53	0.73
1:B:335:THR:OG1	1:B:336:ALA:N	2.20	0.73
1:M:268:PHE:HB2	1:M:365:GLN:HG3	1.71	0.73
1:A:298:ALA:HB3	1:A:347:ILE:HG21	1.71	0.73
1:D:122:ASN:HB3	1:D:218:THR:HG21	1.70	0.72
1:H:295:VAL:C	1:H:296:TRP:CD1	2.61	0.72
1:E:298:ALA:HB3	1:E:347:ILE:HG21	1.71	0.72
1:G:108:THR:HG23	1:G:113:LEU:HD22	1.70	0.72
1:P:109:ASN:H	1:P:240:THR:HB	1.56	0.71
1:G:268:PHE:HB2	1:G:365:GLN:HG3	1.72	0.71
1:D:268:PHE:HB2	1:D:365:GLN:HG3	1.72	0.71
1:N:298:ALA:HB3	1:N:347:ILE:HG21	1.71	0.71
1:B:348:ARG:HG2	1:B:349:VAL:HG12	1.71	0.71
1:I:348:ARG:O	1:I:350:ASN:N	2.24	0.71
1:H:296:TRP:HZ3	1:H:366:LEU:CB	2.01	0.70
1:B:348:ARG:O	1:B:350:ASN:N	2.25	0.70
1:H:298:ALA:HB3	1:H:347:ILE:HG21	1.73	0.70
1:O:109:ASN:H	1:O:240:THR:HB	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:298:ALA:HB3	1:K:347:ILE:HG21	1.73	0.69
1:J:210:ASN:O	1:J:210:ASN:OD1	2.09	0.69
1:F:121:ASN:HB3	1:F:230:GLN:OE1	1.92	0.69
1:P:268:PHE:HB2	1:P:365:GLN:HG3	1.73	0.69
1:I:159:LEU:HB2	1:I:244:GLY:HA2	1.74	0.69
1:I:348:ARG:HG3	1:I:349:VAL:HG12	1.74	0.69
1:A:269:ARG:NH2	1:A:271:SER:OG	2.26	0.69
1:O:348:ARG:HG2	1:O:349:VAL:HG12	1.72	0.69
1:A:268:PHE:HB2	1:A:365:GLN:HG3	1.73	0.69
1:D:297:GLN:OE1	1:D:299:ARG:NH1	2.24	0.68
1:F:348:ARG:O	1:F:350:ASN:N	2.26	0.68
1:H:99[B]:ARG:NH2	4:H:502:HOH:O	2.25	0.68
1:B:109:ASN:H	1:B:240:THR:HB	1.57	0.68
1:E:269:ARG:NH2	1:E:271:SER:OG	2.26	0.68
1:O:348:ARG:O	1:O:350:ASN:N	2.26	0.68
1:M:297:GLN:OE1	1:M:299:ARG:NH1	2.26	0.68
1:E:268:PHE:HB2	1:E:365:GLN:HG3	1.74	0.68
1:N:268:PHE:HB2	1:N:365:GLN:HG3	1.76	0.67
1:D:165:ASN:HB3	1:O:161:ASN:HB3	1.76	0.67
1:D:108:THR:HG23	1:D:113:LEU:HD22	1.75	0.67
1:J:268:PHE:HB2	1:J:365:GLN:HG3	1.75	0.67
1:F:161:ASN:HB3	1:J:165:ASN:HB3	1.75	0.67
1:J:108:THR:HG23	1:J:113:LEU:HD22	1.76	0.67
1:L:348:ARG:O	1:L:350:ASN:N	2.28	0.67
1:P:297:GLN:OE1	1:P:299:ARG:NH1	2.26	0.67
1:B:159:LEU:HB2	1:B:244:GLY:HA2	1.77	0.67
1:K:268:PHE:HB2	1:K:365:GLN:HG3	1.75	0.67
1:H:192:HIS:NE2	1:I:256:GLU:OE2	2.25	0.66
1:D:109:ASN:H	1:D:240:THR:HB	1.61	0.66
1:A:296:TRP:N	1:A:296:TRP:CD1	2.63	0.66
1:E:196:ILE:HG12	1:E:202:THR:HB	1.78	0.66
1:E:296:TRP:CD1	1:E:296:TRP:N	2.62	0.66
1:H:268:PHE:HB2	1:H:365:GLN:HG3	1.77	0.66
1:M:108:THR:HG23	1:M:113:LEU:HD22	1.77	0.66
1:N:296:TRP:N	1:N:296:TRP:CD1	2.64	0.65
1:H:278:ARG:NH1	1:H:280:GLY:O	2.30	0.65
1:K:296:TRP:CD1	1:K:296:TRP:N	2.61	0.65
1:H:196:ILE:HG12	1:H:202:THR:HB	1.78	0.65
1:J:297:GLN:OE1	1:J:299:ARG:NH1	2.29	0.64
1:P:108:THR:HG23	1:P:113:LEU:HD22	1.78	0.64
1:O:159:LEU:HB2	1:O:244:GLY:HA2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:109:ASN:H	1:L:240:THR:HB	1.63	0.64
1:B:318:THR:OG1	1:B:357:GLY:N	2.22	0.64
1:A:196:ILE:HG12	1:A:202:THR:HB	1.78	0.64
1:F:318:THR:OG1	1:F:357:GLY:N	2.21	0.64
1:N:269:ARG:NH2	1:N:271:SER:OG	2.31	0.64
1:H:296:TRP:HB2	1:H:353:LEU:CD2	2.27	0.64
1:K:196:ILE:HG12	1:K:202:THR:HB	1.80	0.64
1:A:278:ARG:NH1	1:A:280:GLY:O	2.31	0.64
1:K:109:ASN:H	1:K:240:THR:HB	1.63	0.64
1:B:318:THR:HB	1:B:356:SER:HB2	1.78	0.63
1:K:269:ARG:NH2	1:K:271:SER:OG	2.31	0.63
1:K:192:HIS:NE2	1:L:256:GLU:OE2	2.28	0.63
1:F:318:THR:HB	1:F:356:SER:HB2	1.79	0.63
1:L:318:THR:OG1	1:L:357:GLY:N	2.23	0.63
1:N:192:HIS:NE2	1:O:256:GLU:OE2	2.28	0.63
1:O:318:THR:HB	1:O:356:SER:HB2	1.80	0.63
1:E:278:ARG:NH1	1:E:280:GLY:O	2.30	0.63
1:I:318:THR:OG1	1:I:357:GLY:N	2.22	0.63
1:K:278:ARG:NH1	1:K:280:GLY:O	2.32	0.63
1:N:196:ILE:HG12	1:N:202:THR:HB	1.80	0.63
1:O:288:VAL:H	1:O:295:VAL:HG23	1.62	0.63
1:I:161:ASN:HB3	1:M:165:ASN:HB3	1.81	0.62
1:L:161:ASN:HB3	1:P:165:ASN:HB3	1.81	0.62
1:G:297:GLN:OE1	1:G:299:ARG:NH1	2.30	0.62
1:I:318:THR:HB	1:I:356:SER:HB2	1.81	0.62
1:D:314:VAL:HG22	1:D:315:GLY:H	1.64	0.62
1:H:269:ARG:NH2	1:H:271:SER:OG	2.33	0.62
1:B:288:VAL:H	1:B:295:VAL:HG23	1.65	0.62
1:L:288:VAL:H	1:L:295:VAL:HG23	1.64	0.62
1:L:159:LEU:HB2	1:L:244:GLY:HA2	1.81	0.62
1:O:358:LEU:HD23	1:O:361:ALA:HB2	1.82	0.61
1:A:192:HIS:NE2	1:B:256:GLU:OE2	2.30	0.61
1:I:348:ARG:NH2	4:I:501:HOH:O	2.33	0.61
1:G:122:ASN:HB3	1:G:218:THR:HG21	1.84	0.60
1:I:118:THR:O	1:I:120:PRO:HD2	2.02	0.60
1:F:288:VAL:H	1:F:295:VAL:HG23	1.65	0.60
1:F:118:THR:O	1:F:120:PRO:HD2	2.01	0.60
1:I:109:ASN:H	1:I:240:THR:HB	1.66	0.60
1:D:288:VAL:HG22	1:D:295:VAL:HG22	1.83	0.60
1:K:362:THR:OG1	1:K:363:ASN:N	2.34	0.60
1:F:159:LEU:HB2	1:F:244:GLY:HA2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:122:ASN:HB3	1:P:218:THR:HG21	1.84	0.60
1:I:348:ARG:HG3	1:I:349:VAL:N	2.15	0.60
1:K:129:LEU:HD22	1:K:138:VAL:HG23	1.82	0.60
1:J:288:VAL:HG22	1:J:295:VAL:HG22	1.83	0.60
1:L:358:LEU:HD23	1:L:361:ALA:HB2	1.82	0.60
1:P:288:VAL:HG22	1:P:295:VAL:HG22	1.82	0.60
1:N:134:PHE:HB3	1:N:137:LEU:HB3	1.84	0.60
1:B:161:ASN:HB3	1:G:165:ASN:HB3	1.83	0.60
1:M:288:VAL:HG22	1:M:295:VAL:HG22	1.84	0.60
1:E:134:PHE:HB3	1:E:137:LEU:HB3	1.84	0.60
1:H:296:TRP:CZ3	1:H:366:LEU:CB	2.67	0.60
1:O:371:ALA:HB1	1:O:375:ASN:OD1	2.02	0.60
1:B:118:THR:O	1:B:120:PRO:HD2	2.01	0.60
1:O:318:THR:OG1	1:O:357:GLY:N	2.21	0.59
1:H:321:ILE:HG21	1:H:325:GLY:HA3	1.84	0.59
1:I:176:SER:HA	1:I:230:GLN:HB2	1.83	0.59
1:G:99[A]:ARG:HG2	1:G:99[A]:ARG:HH11	1.67	0.59
1:B:153:ARG:HD3	1:B:205:THR:HG23	1.84	0.59
1:N:278:ARG:NH1	1:N:280:GLY:O	2.36	0.59
1:K:134:PHE:HB3	1:K:137:LEU:HB3	1.83	0.59
1:O:118:THR:O	1:O:120:PRO:HD2	2.02	0.59
1:L:118:THR:O	1:L:120:PRO:HD2	2.02	0.58
1:A:134:PHE:HB3	1:A:137:LEU:HB3	1.83	0.58
1:E:182:ASP:OD1	1:H:373:THR:OG1	2.18	0.58
1:B:176:SER:HA	1:B:230:GLN:HB2	1.84	0.58
1:E:113:LEU:HD21	1:E:116:ASN:HA	1.84	0.58
1:H:296:TRP:HE3	1:H:366:LEU:CD2	2.04	0.58
1:M:99[A]:ARG:HG2	1:M:99[A]:ARG:HH11	1.69	0.58
1:H:134:PHE:HB3	1:H:137:LEU:HB3	1.85	0.58
1:P:93:SER:HB3	1:P:255:PHE:CE1	2.38	0.58
1:E:192:HIS:NE2	1:F:256:GLU:OE2	2.30	0.58
1:O:176:SER:HA	1:O:230:GLN:HB2	1.86	0.58
1:P:314:VAL:HG22	1:P:315:GLY:H	1.68	0.57
1:G:288:VAL:HG22	1:G:295:VAL:HG22	1.87	0.57
1:H:109:ASN:H	1:H:240:THR:HB	1.69	0.57
1:L:176:SER:HA	1:L:230:GLN:HB2	1.85	0.57
1:M:122:ASN:HB3	1:M:218:THR:HG21	1.86	0.57
1:J:99[A]:ARG:HG2	1:J:99[A]:ARG:HH11	1.70	0.57
1:M:312:SER:HA	1:M:361:ALA:HA	1.86	0.57
1:M:314:VAL:HG22	1:M:315:GLY:H	1.70	0.57
1:O:347:ILE:HG13	1:O:351:ALA:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:296:TRP:HB2	1:H:353:LEU:HD23	1.86	0.56
1:L:128:PRO:O	1:L:141:ALA:HB1	2.05	0.56
1:F:371:ALA:HB1	1:F:375:ASN:OD1	2.06	0.56
1:M:93:SER:HB3	1:M:255:PHE:CE1	2.40	0.56
1:A:109:ASN:H	1:A:240:THR:HB	1.70	0.56
1:A:113:LEU:HD21	1:A:116:ASN:HA	1.87	0.56
1:N:109:ASN:H	1:N:240:THR:HB	1.69	0.56
1:A:372:ILE:HD12	1:A:374:GLU:HG2	1.87	0.56
1:B:371:ALA:HB1	1:B:375:ASN:OD1	2.05	0.56
1:P:99[A]:ARG:HH11	1:P:99[A]:ARG:HG2	1.70	0.56
1:B:336:ALA:O	1:B:338:SER:N	2.37	0.56
1:I:371:ALA:HB1	1:I:375:ASN:OD1	2.06	0.56
1:G:312:SER:HA	1:G:361:ALA:HA	1.87	0.56
1:I:336:ALA:O	1:I:338:SER:N	2.39	0.55
1:F:176:SER:HA	1:F:230:GLN:HB2	1.87	0.55
1:G:314:VAL:HG22	1:G:315:GLY:H	1.70	0.55
1:M:127:ASN:HB2	1:M:227:ASN:OD1	2.06	0.55
1:N:129:LEU:HD22	1:N:138:VAL:HG23	1.88	0.55
1:K:113:LEU:HD21	1:K:116:ASN:HA	1.88	0.55
1:N:321:ILE:HG21	1:N:325:GLY:HA3	1.87	0.55
1:L:371:ALA:HB1	1:L:375:ASN:OD1	2.05	0.55
1:A:321:ILE:HG21	1:A:325:GLY:HA3	1.89	0.55
1:I:120:PRO:O	1:I:122:ASN:N	2.37	0.55
1:N:362:THR:OG1	1:N:363:ASN:N	2.38	0.55
1:N:372:ILE:HD12	1:N:374:GLU:HG2	1.88	0.55
1:E:321:ILE:HG21	1:E:325:GLY:HA3	1.89	0.55
1:G:114:ARG:HE	1:G:120:PRO:HD3	1.72	0.55
1:I:288:VAL:H	1:I:295:VAL:HG23	1.72	0.55
1:P:105:LEU:HG	1:P:233:TRP:CD1	2.42	0.55
1:K:321:ILE:HG21	1:K:325:GLY:HA3	1.88	0.55
1:A:105:LEU:HG	1:A:233:TRP:CD1	2.42	0.55
1:J:93:SER:HB3	1:J:255:PHE:CE1	2.42	0.54
1:E:109:ASN:H	1:E:240:THR:HB	1.72	0.54
1:J:127:ASN:HB2	1:J:227:ASN:OD1	2.07	0.54
1:A:129:LEU:HD22	1:A:138:VAL:HG23	1.88	0.54
1:F:336:ALA:O	1:F:338:SER:N	2.38	0.54
1:O:336:ALA:O	1:O:338:SER:N	2.39	0.54
1:K:288:VAL:HG22	1:K:295:VAL:HG22	1.90	0.54
1:N:113:LEU:HD21	1:N:116:ASN:HA	1.90	0.54
1:A:347:ILE:HG23	1:A:351:ALA:HB3	1.88	0.54
1:A:150:ASN:O	1:A:208:THR:HG21	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:182:ASP:OD1	1:N:373:THR:OG1	2.23	0.54
1:A:373:THR:OG1	1:N:182:ASP:OD1	2.25	0.54
1:K:105:LEU:HD12	1:K:246:ILE:HD11	1.89	0.54
1:H:113:LEU:HD21	1:H:116:ASN:HA	1.88	0.54
1:E:181:PRO:HG3	1:E:187:LEU:HD23	1.90	0.54
1:H:105:LEU:HG	1:H:233:TRP:CD1	2.42	0.54
1:J:312:SER:HA	1:J:361:ALA:HA	1.90	0.54
1:D:312:SER:HA	1:D:361:ALA:HA	1.89	0.54
1:P:312:SER:HA	1:P:361:ALA:HA	1.89	0.54
1:D:99[A]:ARG:HG2	1:D:99[A]:ARG:HH11	1.73	0.54
1:K:150:ASN:O	1:K:208:THR:HG21	2.08	0.54
1:O:358:LEU:HD23	1:O:361:ALA:CB	2.38	0.53
1:L:358:LEU:HD23	1:L:361:ALA:CB	2.38	0.53
1:G:93:SER:HB3	1:G:255:PHE:CE1	2.42	0.53
1:E:129:LEU:HD22	1:E:138:VAL:HG23	1.90	0.53
1:N:108:THR:HG23	1:N:113:LEU:HD13	1.89	0.53
1:B:134:PHE:HB3	1:B:137:LEU:HB3	1.90	0.53
1:E:150:ASN:O	1:E:208:THR:HG21	2.09	0.53
1:O:120:PRO:O	1:O:122:ASN:N	2.39	0.53
1:G:159:LEU:HB2	1:G:244:GLY:HA2	1.91	0.53
1:D:93:SER:HB3	1:D:255:PHE:CE1	2.44	0.53
1:B:120:PRO:O	1:B:122:ASN:N	2.40	0.53
1:D:127:ASN:HB2	1:D:227:ASN:OD1	2.08	0.53
1:P:159:LEU:HB2	1:P:244:GLY:HA2	1.91	0.53
1:H:260:THR:HG22	1:H:261:SER:O	2.09	0.52
1:J:114:ARG:HE	1:J:120:PRO:HD3	1.73	0.52
1:G:105:LEU:HG	1:G:233:TRP:CD1	2.44	0.52
1:L:336:ALA:O	1:L:338:SER:N	2.40	0.52
1:L:120:PRO:O	1:L:122:ASN:N	2.38	0.52
1:N:347:ILE:HG23	1:N:351:ALA:HB3	1.92	0.52
1:M:105:LEU:HG	1:M:233:TRP:CD1	2.45	0.52
1:H:129:LEU:HD22	1:H:138:VAL:HG23	1.92	0.52
1:E:107:GLY:HA2	1:E:113:LEU:HD22	1.92	0.52
1:N:107:GLY:HA2	1:N:113:LEU:HD22	1.91	0.52
1:P:126:ILE:HD13	1:P:152:LEU:HD21	1.91	0.52
1:D:105:LEU:HG	1:D:233:TRP:CD1	2.45	0.52
1:J:267:LEU:HD13	1:J:278:ARG:HB2	1.92	0.52
1:K:107:GLY:HA2	1:K:113:LEU:HD22	1.92	0.52
1:L:372:ILE:HD11	1:N:262:PRO:HG3	1.92	0.52
1:D:99[B]:ARG:NH2	1:D:155:GLU:OE1	2.43	0.52
1:P:127:ASN:HB2	1:P:227:ASN:OD1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:114:ARG:HE	1:M:120:PRO:HD3	1.73	0.52
1:I:372:ILE:HD12	1:I:374:GLU:HG2	1.92	0.52
1:J:105:LEU:HG	1:J:233:TRP:CD1	2.45	0.52
1:A:260:THR:HG22	1:A:261:SER:O	2.10	0.52
1:G:127:ASN:HB2	1:G:227:ASN:OD1	2.09	0.52
1:D:126:ILE:HD13	1:D:152:LEU:HD21	1.92	0.52
1:F:134:PHE:HB3	1:F:137:LEU:HB3	1.92	0.52
1:F:120:PRO:O	1:F:122:ASN:N	2.38	0.52
1:P:267:LEU:HD13	1:P:278:ARG:HB2	1.92	0.52
1:O:209:ASP:OD2	1:O:213:ARG:NH2	2.37	0.52
1:D:159:LEU:HB2	1:D:244:GLY:HA2	1.92	0.52
1:A:105:LEU:HD12	1:A:246:ILE:HD11	1.92	0.51
1:I:134:PHE:HB3	1:I:137:LEU:HB3	1.91	0.51
1:J:109:ASN:N	1:J:240:THR:HB	2.21	0.51
1:A:269:ARG:HG3	1:A:276:GLN:HB3	1.92	0.51
1:O:134:PHE:HB3	1:O:137:LEU:HB3	1.91	0.51
1:N:105:LEU:HG	1:N:233:TRP:CD1	2.45	0.51
1:E:105:LEU:HG	1:E:233:TRP:CD1	2.45	0.51
1:P:331:PHE:CD2	1:P:379:VAL:HG23	2.44	0.51
1:L:320:SER:HG	1:L:354:SER:HG	1.58	0.51
1:D:114:ARG:HE	1:D:120:PRO:HD3	1.76	0.51
1:H:347:ILE:HG23	1:H:351:ALA:HB3	1.91	0.51
1:B:358:LEU:HD23	1:B:361:ALA:HB2	1.93	0.51
1:L:134:PHE:HB3	1:L:137:LEU:HB3	1.91	0.51
1:M:126:ILE:HD13	1:M:152:LEU:HD21	1.92	0.51
1:D:175:ASP:HB3	1:D:178:ASP:HB2	1.93	0.51
1:I:143:ASN:HB3	1:K:136:TRP:CZ2	2.46	0.51
1:F:109:ASN:N	1:F:240:THR:HB	2.25	0.51
1:M:99[B]:ARG:NH2	1:M:155:GLU:OE1	2.44	0.51
1:B:124:PHE:CE1	1:B:132:PHE:HE2	2.29	0.51
1:H:108:THR:HG23	1:H:113:LEU:HD13	1.92	0.51
1:G:126:ILE:HD13	1:G:152:LEU:HD21	1.93	0.50
1:H:181:PRO:HG3	1:H:187:LEU:HD23	1.93	0.50
1:F:153:ARG:HD3	1:F:205:THR:HG23	1.92	0.50
1:M:301:PRO:HD3	1:M:349:VAL:HG22	1.93	0.50
1:E:105:LEU:HD12	1:E:246:ILE:HD11	1.93	0.50
1:L:260:THR:HG22	1:L:261:SER:O	2.10	0.50
1:B:358:LEU:HD23	1:B:361:ALA:CB	2.41	0.50
1:F:303:THR:HB	1:F:371:ALA:O	2.12	0.50
1:K:105:LEU:HG	1:K:233:TRP:CD1	2.46	0.50
1:G:331:PHE:CD2	1:G:379:VAL:HG23	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:269:ARG:HG3	1:K:276:GLN:HB3	1.93	0.50
1:J:99[B]:ARG:NH2	1:J:155:GLU:OE1	2.45	0.50
1:I:124:PHE:CE1	1:I:132:PHE:HE2	2.30	0.50
1:E:372:ILE:HD12	1:E:374:GLU:HG2	1.93	0.50
1:M:147:TYR:OH	1:M:226:ILE:O	2.20	0.50
1:M:331:PHE:CD2	1:M:379:VAL:HG23	2.47	0.50
1:B:266:SER:HB3	1:E:375:ASN:HD22	1.77	0.50
1:D:331:PHE:CD1	1:D:379:VAL:HG23	2.46	0.50
1:O:124:PHE:CE1	1:O:132:PHE:HE2	2.29	0.50
1:F:107:GLY:HA2	1:F:113:LEU:HD23	1.93	0.50
1:G:109:ASN:N	1:G:240:THR:HB	2.25	0.49
1:K:313:THR:O	1:K:314:VAL:HG12	2.11	0.49
1:N:269:ARG:HG3	1:N:276:GLN:HB3	1.93	0.49
1:K:108:THR:HG23	1:K:113:LEU:HD13	1.94	0.49
1:N:150:ASN:O	1:N:208:THR:HG21	2.11	0.49
1:F:292:THR:O	1:F:358:LEU:HB2	2.11	0.49
1:J:175:ASP:HB3	1:J:178:ASP:HB2	1.93	0.49
1:F:99[A]:ARG:HD2	1:F:249:GLU:OE1	2.12	0.49
1:A:182:ASP:OD1	1:E:373:THR:OG1	2.23	0.49
1:L:318:THR:HB	1:L:356:SER:HB2	1.94	0.49
1:L:321:ILE:HA	1:L:352:ASN:O	2.12	0.49
1:F:124:PHE:CE1	1:F:132:PHE:HE2	2.30	0.49
1:K:347:ILE:HG23	1:K:351:ALA:HB3	1.94	0.49
1:N:105:LEU:HD12	1:N:246:ILE:HD11	1.94	0.49
1:K:181:PRO:HG3	1:K:187:LEU:HD23	1.95	0.49
1:J:331:PHE:CD1	1:J:379:VAL:HG23	2.47	0.49
1:I:136:TRP:CZ2	1:K:143:ASN:HB3	2.48	0.49
1:N:299:ARG:NH2	4:N:503:HOH:O	2.45	0.49
1:E:108:THR:HG23	1:E:113:LEU:HD13	1.94	0.49
1:H:107:GLY:HA2	1:H:113:LEU:HD22	1.94	0.49
1:I:292:THR:O	1:I:358:LEU:HB2	2.13	0.49
1:O:99[A]:ARG:HD2	1:O:249:GLU:OE1	2.13	0.49
1:E:167:ARG:NH2	1:H:159:LEU:HD13	2.28	0.49
1:A:107:GLY:HA2	1:A:113:LEU:HD22	1.94	0.49
1:I:372:ILE:HG13	1:I:375:ASN:OD1	2.13	0.49
1:F:372:ILE:HD11	1:H:262:PRO:HG3	1.94	0.48
1:N:167:ARG:HD2	1:N:195:GLU:HB3	1.94	0.48
1:A:136:TRP:CZ2	1:O:143:ASN:HB3	2.47	0.48
1:E:298:ALA:CB	1:E:347:ILE:HG21	2.41	0.48
1:E:347:ILE:HG23	1:E:351:ALA:HB3	1.94	0.48
1:J:295:VAL:HG12	1:J:354:SER:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:PRO:HG3	1:O:372:ILE:HD11	1.95	0.48
1:I:320:SER:HG	1:I:354:SER:HG	1.59	0.48
1:L:294:LEU:HB2	1:L:355:LEU:HB2	1.96	0.48
1:F:143:ASN:HB3	1:H:136:TRP:CZ2	2.48	0.48
1:B:260:THR:HG22	1:B:261:SER:O	2.14	0.48
1:P:114:ARG:HE	1:P:120:PRO:HD3	1.78	0.48
1:N:181:PRO:HG3	1:N:187:LEU:HD23	1.95	0.48
1:O:121:ASN:HB3	1:O:230:GLN:OE1	2.13	0.48
1:H:105:LEU:HD12	1:H:246:ILE:HD11	1.95	0.48
1:I:153:ARG:HD3	1:I:205:THR:HG23	1.96	0.48
1:G:99[B]:ARG:NH2	1:G:155:GLU:OE1	2.45	0.48
1:L:303:THR:HB	1:L:371:ALA:O	2.13	0.48
1:B:311:ASN:O	1:B:361:ALA:HA	2.13	0.48
1:L:124:PHE:CE1	1:L:132:PHE:HE2	2.31	0.48
1:K:372:ILE:HD12	1:K:374:GLU:HG2	1.95	0.48
1:P:134:PHE:HB3	1:P:137:LEU:HB3	1.95	0.48
1:D:271:SER:HA	1:D:272:ALA:HA	1.62	0.48
1:K:298:ALA:CB	1:K:347:ILE:HG21	2.42	0.48
1:H:372:ILE:HD12	1:H:374:GLU:HG2	1.96	0.47
1:A:108:THR:HG23	1:A:113:LEU:HD13	1.95	0.47
1:L:153:ARG:HD3	1:L:205:THR:HG23	1.95	0.47
1:H:269:ARG:HG3	1:H:276:GLN:HB3	1.97	0.47
1:B:99[A]:ARG:HD2	1:B:249:GLU:OE1	2.14	0.47
1:A:181:PRO:HG3	1:A:187:LEU:HD23	1.95	0.47
1:B:114:ARG:HD2	1:B:181:PRO:HD2	1.96	0.47
1:I:266:SER:HB3	1:K:375:ASN:HD22	1.77	0.47
1:D:301:PRO:HD3	1:D:349:VAL:HG22	1.95	0.47
1:M:121:ASN:HD21	1:M:299:ARG:HE	1.62	0.47
1:P:121:ASN:HD21	1:P:299:ARG:HE	1.61	0.47
1:M:159:LEU:HB2	1:M:244:GLY:HA2	1.96	0.47
1:L:266:SER:HB3	1:N:375:ASN:HD22	1.79	0.47
1:J:159:LEU:HB2	1:J:244:GLY:HA2	1.97	0.47
1:A:294:LEU:HA	1:A:294:LEU:HD12	1.78	0.47
1:L:292:THR:O	1:L:358:LEU:HB2	2.15	0.47
1:L:299:ARG:NH2	4:L:404:HOH:O	2.39	0.47
1:D:81:LYS:O	1:D:99[A]:ARG:NH2	2.47	0.47
1:M:175:ASP:HB3	1:M:178:ASP:HB2	1.97	0.47
1:D:91:LYS:HD2	1:D:91:LYS:HA	1.67	0.47
1:I:161:ASN:O	1:I:199:TRP:HB3	2.15	0.47
1:L:143:ASN:HB3	1:N:136:TRP:CZ2	2.50	0.47
1:G:134:PHE:HB3	1:G:137:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:THR:HG22	1:E:261:SER:O	2.14	0.47
1:O:292:THR:O	1:O:358:LEU:HB2	2.15	0.47
1:N:260:THR:HG22	1:N:261:SER:O	2.15	0.47
1:H:150:ASN:O	1:H:208:THR:HG21	2.15	0.47
1:G:295:VAL:HG12	1:G:354:SER:HB2	1.97	0.47
1:B:303:THR:HB	1:B:371:ALA:O	2.15	0.47
1:I:311:ASN:O	1:I:361:ALA:HA	2.15	0.47
1:B:113:LEU:HD12	1:B:113:LEU:HA	1.75	0.47
1:B:136:TRP:CZ2	1:E:143:ASN:HB3	2.50	0.47
1:P:129:LEU:HD22	1:P:129:LEU:HA	1.70	0.47
1:B:109:ASN:N	1:B:240:THR:HB	2.27	0.46
1:D:109:ASN:N	1:D:240:THR:HB	2.28	0.46
1:P:99[B]:ARG:NH2	1:P:155:GLU:OE1	2.47	0.46
1:G:134:PHE:O	1:G:138:VAL:HG23	2.15	0.46
1:G:267:LEU:HD13	1:G:278:ARG:HB2	1.97	0.46
1:O:303:THR:HB	1:O:371:ALA:O	2.15	0.46
1:G:114:ARG:HD2	1:G:181:PRO:HD2	1.97	0.46
1:J:95:ARG:NH2	1:J:150:ASN:HD21	2.13	0.46
1:G:91:LYS:HD2	1:G:91:LYS:HA	1.63	0.46
1:P:312:SER:O	1:P:337:GLY:HA2	2.16	0.46
1:D:290:SER:OG	1:D:291:ALA:N	2.48	0.46
1:B:143:ASN:HB3	1:E:136:TRP:CZ2	2.51	0.46
1:J:134:PHE:HB3	1:J:137:LEU:HB3	1.98	0.46
1:B:372:ILE:HG13	1:B:375:ASN:OD1	2.15	0.46
1:L:286:LEU:HD13	1:L:296:TRP:CZ3	2.51	0.46
1:A:313:THR:O	1:A:314:VAL:HG12	2.15	0.46
1:O:114:ARG:HD2	1:O:181:PRO:HD2	1.97	0.46
1:M:109:ASN:N	1:M:240:THR:HB	2.25	0.46
1:F:161:ASN:N	1:J:165:ASN:HB3	2.30	0.46
1:J:312:SER:O	1:J:337:GLY:HA2	2.14	0.46
1:G:175:ASP:HB3	1:G:178:ASP:HB2	1.97	0.46
1:M:263:LEU:HD22	1:M:281:LEU:HD11	1.97	0.46
1:P:175:ASP:HB3	1:P:178:ASP:HB2	1.98	0.46
1:E:370:ARG:HD3	1:E:370:ARG:HA	1.61	0.46
1:D:165:ASN:HD22	1:O:161:ASN:HD22	1.64	0.46
1:I:108:THR:HG23	1:I:113:LEU:HD22	1.97	0.46
1:D:196:ILE:HD13	1:D:202:THR:HB	1.98	0.46
1:G:95:ARG:HG3	1:G:253:ASP:OD1	2.16	0.46
1:J:81:LYS:O	1:J:99[A]:ARG:NH2	2.49	0.46
1:H:313:THR:O	1:H:314:VAL:HG12	2.16	0.46
1:E:269:ARG:HG3	1:E:276:GLN:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ILE:HD11	1:E:262:PRO:HG3	1.97	0.46
1:J:301:PRO:HD3	1:J:349:VAL:HG22	1.98	0.46
1:M:134:PHE:HB3	1:M:137:LEU:HB3	1.98	0.46
1:L:120:PRO:HG2	4:L:404:HOH:O	2.15	0.46
1:G:301:PRO:HD3	1:G:349:VAL:HG22	1.98	0.46
1:J:126:ILE:HD13	1:J:152:LEU:HD21	1.98	0.46
1:D:134:PHE:HB3	1:D:137:LEU:HB3	1.98	0.46
1:N:298:ALA:CB	1:N:347:ILE:HG21	2.42	0.45
1:J:121:ASN:HD21	1:J:299:ARG:HE	1.64	0.45
1:L:161:ASN:N	1:P:165:ASN:HB3	2.31	0.45
1:G:105:LEU:HD12	1:G:246:ILE:HD11	1.97	0.45
1:N:313:THR:O	1:N:314:VAL:HG12	2.16	0.45
1:J:196:ILE:HG21	1:J:202:THR:HB	1.98	0.45
1:L:108:THR:HG23	1:L:113:LEU:HD22	1.98	0.45
1:I:123:ASP:OD1	1:I:123:ASP:N	2.47	0.45
1:P:109:ASN:N	1:P:240:THR:HB	2.26	0.45
1:O:260:THR:HG22	1:O:261:SER:O	2.16	0.45
1:I:303:THR:HB	1:I:371:ALA:O	2.17	0.45
1:D:312:SER:O	1:D:337:GLY:HA2	2.15	0.45
1:D:165:ASN:HB3	1:O:161:ASN:N	2.32	0.45
1:J:60:ILE:HG21	1:J:60:ILE:HD13	1.35	0.45
1:B:271:SER:HA	1:B:272:ALA:HA	1.79	0.45
1:K:157:VAL:HA	1:K:158:PRO:HD3	1.77	0.45
1:K:370:ARG:HA	1:K:370:ARG:HD3	1.63	0.45
1:M:298:ALA:HB2	1:M:347:ILE:HD13	1.98	0.45
1:G:60:ILE:HG22	1:G:61:ALA:N	2.32	0.45
1:D:267:LEU:HD13	1:D:278:ARG:HB2	1.98	0.45
1:E:157:VAL:HA	1:E:158:PRO:HD3	1.80	0.45
1:N:157:VAL:HA	1:N:158:PRO:HD3	1.77	0.45
1:A:375:ASN:HD22	1:O:266:SER:HB3	1.82	0.45
1:O:107:GLY:HA2	1:O:113:LEU:HD23	1.99	0.45
1:E:288:VAL:HG22	1:E:295:VAL:HG13	1.99	0.45
1:F:283:TYR:OH	1:F:370:ARG:NH2	2.49	0.45
1:E:313:THR:O	1:E:314:VAL:HG12	2.16	0.45
1:N:291:ALA:HB1	1:N:360:GLY:HA2	1.99	0.45
1:M:60:ILE:HG21	1:M:60:ILE:HD13	1.28	0.45
1:L:99[A]:ARG:HD2	1:L:249:GLU:OE1	2.16	0.45
1:H:298:ALA:CB	1:H:347:ILE:HG21	2.45	0.45
1:G:121:ASN:HD21	1:G:299:ARG:HE	1.64	0.45
1:B:347:ILE:HG13	1:B:351:ALA:HB3	1.99	0.45
1:G:271:SER:HA	1:G:272:ALA:HA	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:307:THR:HB	1:M:367:PHE:HB2	1.99	0.45
1:I:347:ILE:HG13	1:I:351:ALA:HB3	1.99	0.45
1:H:256:GLU:OE1	1:J:192:HIS:NE2	2.49	0.44
1:M:264:LEU:HD23	1:M:264:LEU:H	1.81	0.44
1:P:142:ALA:HB2	1:P:263:LEU:HD21	1.98	0.44
1:K:260:THR:HG22	1:K:261:SER:O	2.17	0.44
1:E:109:ASN:N	1:E:240:THR:HB	2.32	0.44
1:L:296:TRP:NE1	1:L:308:ILE:HD13	2.32	0.44
1:I:296:TRP:NE1	1:I:308:ILE:HD13	2.32	0.44
1:A:167:ARG:HD2	1:A:195:GLU:HB3	1.98	0.44
1:F:313:THR:OG1	1:F:313:THR:O	2.34	0.44
1:N:271:SER:HA	1:N:272:ALA:HA	1.71	0.44
1:K:109:ASN:N	1:K:240:THR:HB	2.30	0.44
1:O:318:THR:CB	1:O:356:SER:HB2	2.47	0.44
1:G:263:LEU:HD22	1:G:281:LEU:HD11	1.99	0.44
1:O:294:LEU:HB2	1:O:355:LEU:HB2	2.00	0.44
1:O:311:ASN:O	1:O:361:ALA:HA	2.18	0.44
1:J:196:ILE:HD13	1:J:202:THR:HB	2.00	0.44
1:K:167:ARG:HD2	1:K:195:GLU:HB3	1.99	0.44
1:J:271:SER:HA	1:J:272:ALA:HA	1.61	0.44
1:O:284:PHE:CE1	1:O:298:ALA:HB2	2.53	0.44
1:B:124:PHE:HE1	1:B:233:TRP:CH2	2.34	0.44
1:M:281:LEU:HD12	1:M:283:TYR:OH	2.18	0.44
1:I:99[A]:ARG:HD2	1:I:249:GLU:OE1	2.18	0.44
1:F:209:ASP:OD2	1:F:213:ARG:NH2	2.37	0.44
1:M:129:LEU:HD22	1:M:129:LEU:HA	1.68	0.44
1:E:292:THR:O	1:E:358:LEU:HB2	2.18	0.44
1:K:314:VAL:H	1:K:336:ALA:HA	1.83	0.44
1:F:269:ARG:HE	1:F:289:ALA:HB3	1.83	0.44
1:O:312:SER:HB2	1:O:313:THR:H	1.65	0.44
1:F:114:ARG:HD2	1:F:181:PRO:HD2	1.99	0.44
1:P:264:LEU:HB2	1:P:369:VAL:HG12	1.99	0.44
1:O:271:SER:HA	1:O:272:ALA:HA	1.73	0.44
1:M:114:ARG:HD2	1:M:181:PRO:HD2	1.99	0.44
1:J:225:LEU:HD23	1:J:225:LEU:HA	1.84	0.44
1:I:100:GLU:OE2	1:I:250:TYR:OH	2.26	0.44
1:A:109:ASN:N	1:A:240:THR:HB	2.33	0.44
1:B:347:ILE:HA	1:B:347:ILE:HD12	1.89	0.44
1:P:264:LEU:HD23	1:P:264:LEU:H	1.83	0.44
1:O:224:LYS:HB3	1:P:214:PHE:CE2	2.53	0.44
1:N:370:ARG:HD3	1:N:370:ARG:HA	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:372:ILE:HG13	1:F:375:ASN:OD1	2.18	0.44
1:M:290:SER:OG	1:M:291:ALA:N	2.51	0.44
1:I:270:GLU:HA	1:I:271:SER:HB2	2.00	0.44
1:G:196:ILE:HD13	1:G:202:THR:HB	2.00	0.44
1:F:311:ASN:O	1:F:361:ALA:HA	2.17	0.44
1:L:113:LEU:HD12	1:L:113:LEU:HA	1.75	0.43
1:A:143:ASN:HB3	1:O:136:TRP:CZ2	2.53	0.43
1:I:260:THR:HG22	1:I:261:SER:O	2.18	0.43
1:L:300:VAL:HA	1:L:301:PRO:HD2	1.79	0.43
1:B:158:PRO:HB3	1:B:198:PRO:O	2.18	0.43
1:L:129:LEU:O	1:L:131:PRO:HD3	2.18	0.43
1:M:203:LYS:HB3	1:M:203:LYS:HE2	1.81	0.43
1:I:113:LEU:HA	1:I:113:LEU:HD12	1.81	0.43
1:G:60:ILE:HG21	1:G:60:ILE:HD13	1.51	0.43
1:G:100:GLU:OE2	1:G:136:TRP:HB3	2.18	0.43
1:H:167:ARG:HD2	1:H:195:GLU:HB3	2.00	0.43
1:G:286:LEU:HD13	1:G:296:TRP:CE3	2.53	0.43
1:B:284:PHE:CE2	1:B:298:ALA:HB2	2.53	0.43
1:I:129:LEU:HD22	1:I:129:LEU:HA	1.81	0.43
1:J:290:SER:OG	1:J:291:ALA:N	2.51	0.43
1:J:314:VAL:HG13	1:J:315:GLY:N	2.33	0.43
1:D:313:THR:O	1:D:314:VAL:HG12	2.19	0.43
1:O:307:THR:HB	1:O:367:PHE:HB2	1.99	0.43
1:I:224:LYS:HB3	1:J:214:PHE:CE2	2.53	0.43
1:P:295:VAL:HG12	1:P:354:SER:HB2	1.99	0.43
1:M:295:VAL:HG12	1:M:354:SER:HB2	2.01	0.43
1:N:109:ASN:N	1:N:240:THR:HB	2.32	0.43
1:M:134:PHE:O	1:M:138:VAL:HG23	2.19	0.43
1:O:127:ASN:HB2	1:O:227:ASN:OD1	2.18	0.43
1:J:281:LEU:HD12	1:J:283:TYR:OH	2.18	0.43
1:D:295:VAL:HG12	1:D:354:SER:HB2	2.00	0.43
1:M:267:LEU:HD13	1:M:278:ARG:HB2	2.00	0.43
1:G:312:SER:O	1:G:337:GLY:HA2	2.17	0.43
1:G:313:THR:O	1:G:314:VAL:HG12	2.18	0.43
1:D:134:PHE:O	1:D:138:VAL:HG23	2.17	0.43
1:D:298:ALA:HB2	1:D:347:ILE:HD13	2.01	0.43
1:F:187:LEU:HD22	1:F:193:LEU:HD13	2.01	0.43
1:N:256:GLU:OE1	1:P:192:HIS:NE2	2.50	0.43
1:B:296:TRP:NE1	1:B:308:ILE:HD13	2.34	0.43
1:F:129:LEU:HA	1:F:129:LEU:HD22	1.78	0.43
1:O:372:ILE:HG13	1:O:375:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ARG:HD2	1:D:181:PRO:HD2	2.00	0.43
1:G:310:PHE:CE1	1:G:339:SER:HB2	2.54	0.43
1:M:271:SER:HA	1:M:272:ALA:HA	1.63	0.43
1:F:124:PHE:HE1	1:F:233:TRP:CH2	2.37	0.43
1:N:159:LEU:HD12	1:N:159:LEU:HA	1.83	0.43
1:F:260:THR:HG22	1:F:261:SER:O	2.19	0.43
1:B:294:LEU:HB2	1:B:355:LEU:HB2	2.00	0.43
1:G:290:SER:OG	1:G:291:ALA:N	2.52	0.43
1:M:91:LYS:HA	1:M:91:LYS:HD2	1.67	0.43
1:L:311:ASN:O	1:L:361:ALA:HA	2.19	0.43
1:J:314:VAL:HG13	1:J:315:GLY:H	1.84	0.43
1:M:95:ARG:NH2	1:M:150:ASN:HD21	2.17	0.43
1:M:310:PHE:CE1	1:M:339:SER:HB2	2.54	0.43
1:K:147:TYR:OH	1:K:226:ILE:O	2.25	0.43
1:B:307:THR:HB	1:B:367:PHE:HB2	2.01	0.43
1:B:129:LEU:HD22	1:B:129:LEU:HA	1.85	0.43
1:D:281:LEU:HD12	1:D:283:TYR:OH	2.19	0.43
1:L:159:LEU:HA	1:L:159:LEU:HD12	1.83	0.42
1:J:60:ILE:HG22	1:J:61:ALA:N	2.33	0.42
1:A:329:SER:HB2	1:A:377:VAL:HG13	2.01	0.42
1:I:173:ASP:OD1	1:I:174:LYS:N	2.52	0.42
1:N:292:THR:O	1:N:358:LEU:HB2	2.19	0.42
1:I:294:LEU:HB2	1:I:355:LEU:HB2	2.01	0.42
1:L:348:ARG:CG	1:L:349:VAL:N	2.83	0.42
1:B:348:ARG:CG	1:B:349:VAL:N	2.82	0.42
1:I:209:ASP:OD2	1:I:213:ARG:NH2	2.41	0.42
1:L:136:TRP:CZ2	1:N:143:ASN:HB3	2.54	0.42
1:I:114:ARG:HD2	1:I:181:PRO:HD2	2.01	0.42
1:H:206:VAL:HG23	1:H:207:PRO:HD2	2.02	0.42
1:J:271:SER:HB3	1:J:363:ASN:H	1.84	0.42
1:E:187:LEU:HD22	1:E:187:LEU:O	2.19	0.42
1:G:298:ALA:HB2	1:G:347:ILE:HD13	2.02	0.42
1:M:196:ILE:HG21	1:M:202:THR:HB	2.01	0.42
1:D:162:THR:HA	1:D:199:TRP:CG	2.53	0.42
1:L:372:ILE:HG13	1:L:375:ASN:OD1	2.19	0.42
1:B:107:GLY:HA2	1:B:113:LEU:HD23	2.00	0.42
1:K:188:ALA:HA	1:K:193:LEU:HD22	2.01	0.42
1:O:321:ILE:HA	1:O:352:ASN:O	2.20	0.42
1:K:294:LEU:HA	1:K:294:LEU:HD12	1.80	0.42
1:J:91:LYS:HA	1:J:91:LYS:HD2	1.65	0.42
1:P:196:ILE:HG21	1:P:202:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ASN:HD21	1:D:299:ARG:HE	1.68	0.42
1:K:201:ILE:HG22	1:K:202:THR:N	2.34	0.42
1:G:114:ARG:NE	1:G:120:PRO:HD3	2.34	0.42
1:B:292:THR:O	1:B:358:LEU:HB2	2.19	0.42
1:D:271:SER:HB3	1:D:363:ASN:H	1.84	0.42
1:M:196:ILE:HD13	1:M:202:THR:HB	2.00	0.42
1:F:112:PHE:HE1	1:F:184:ARG:HG2	1.85	0.42
1:E:335:THR:OG1	1:E:336:ALA:N	2.52	0.42
1:D:60:ILE:HG21	1:D:60:ILE:HD13	1.44	0.42
1:A:298:ALA:CB	1:A:347:ILE:HG21	2.43	0.42
1:B:127:ASN:HB2	1:B:227:ASN:OD1	2.19	0.42
1:O:348:ARG:CG	1:O:349:VAL:N	2.83	0.42
1:M:218:THR:HB	1:M:278:ARG:HH22	1.85	0.42
1:M:114:ARG:NE	1:M:120:PRO:HD3	2.35	0.42
1:O:313:THR:O	1:O:313:THR:OG1	2.36	0.42
1:I:172:PHE:CE2	1:I:207:PRO:HD2	2.55	0.42
1:F:321:ILE:HA	1:F:352:ASN:O	2.19	0.42
1:L:307:THR:HB	1:L:367:PHE:HB2	2.01	0.42
1:L:263:LEU:HD23	1:L:263:LEU:HA	1.88	0.42
1:F:348:ARG:CG	1:F:349:VAL:N	2.82	0.42
1:P:218:THR:HB	1:P:278:ARG:HH22	1.85	0.42
1:N:187:LEU:O	1:N:187:LEU:HD22	2.20	0.42
1:P:134:PHE:O	1:P:138:VAL:HG23	2.19	0.42
1:D:196:ILE:HG21	1:D:202:THR:HB	2.01	0.42
1:D:263:LEU:HD22	1:D:281:LEU:HD11	2.00	0.42
1:L:283:TYR:OH	1:L:370:ARG:NH2	2.53	0.42
1:P:271:SER:HA	1:P:272:ALA:HA	1.61	0.42
1:P:95:ARG:HG3	1:P:253:ASP:OD1	2.20	0.42
1:B:276:GLN:OE1	1:B:286:LEU:HB3	2.20	0.42
1:H:370:ARG:HA	1:H:370:ARG:HD3	1.74	0.42
1:O:158:PRO:HB3	1:O:198:PRO:O	2.19	0.42
1:F:335:THR:HG1	1:F:336:ALA:H	1.58	0.42
1:F:94:VAL:HG21	1:H:96:ILE:HD13	2.02	0.42
1:L:183:ASP:OD2	1:L:185:ALA:HB3	2.20	0.42
1:P:273:SER:O	1:P:274:SER:HB2	2.20	0.42
1:M:286:LEU:HD13	1:M:296:TRP:CE3	2.54	0.42
1:L:347:ILE:HG13	1:L:351:ALA:HB3	2.01	0.42
1:A:271:SER:HA	1:A:272:ALA:HA	1.70	0.41
1:G:95:ARG:NH2	1:G:150:ASN:HD21	2.18	0.41
1:P:271:SER:HB3	1:P:363:ASN:H	1.84	0.41
1:P:298:ALA:HB2	1:P:347:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:VAL:HA	1:H:158:PRO:HD3	1.79	0.41
1:F:294:LEU:HB2	1:F:355:LEU:HB2	2.02	0.41
1:B:321:ILE:HA	1:B:352:ASN:O	2.20	0.41
1:L:127:ASN:HB2	1:L:227:ASN:OD1	2.20	0.41
1:A:206:VAL:HG23	1:A:207:PRO:HD2	2.01	0.41
1:G:203:LYS:HE2	1:G:203:LYS:HB3	1.79	0.41
1:L:312:SER:O	1:L:337:GLY:HA2	2.20	0.41
1:O:312:SER:O	1:O:337:GLY:HA2	2.21	0.41
1:L:129:LEU:HD13	1:L:129:LEU:O	2.20	0.41
1:P:290:SER:OG	1:P:291:ALA:N	2.53	0.41
1:I:127:ASN:HB2	1:I:227:ASN:OD1	2.20	0.41
1:F:266:SER:HB3	1:H:375:ASN:HD22	1.85	0.41
1:N:300:VAL:O	1:N:304:TYR:OH	2.32	0.41
1:K:271:SER:HA	1:K:272:ALA:HA	1.73	0.41
1:F:129:LEU:HD13	1:F:129:LEU:O	2.20	0.41
1:F:347:ILE:HG13	1:F:351:ALA:HB3	2.02	0.41
1:B:269:ARG:HE	1:B:289:ALA:HB3	1.85	0.41
1:O:296:TRP:NE1	1:O:308:ILE:HD13	2.36	0.41
1:J:122:ASN:N	1:J:122:ASN:OD1	2.53	0.41
1:H:109:ASN:N	1:H:240:THR:HB	2.32	0.41
1:J:114:ARG:NE	1:J:120:PRO:HD3	2.36	0.41
1:I:269:ARG:HE	1:I:289:ALA:HB3	1.84	0.41
1:N:114:ARG:HG2	1:N:114:ARG:H	1.76	0.41
1:I:299:ARG:HA	1:I:299:ARG:HD2	1.95	0.41
1:G:264:LEU:H	1:G:264:LEU:HD23	1.84	0.41
1:P:286:LEU:HD13	1:P:296:TRP:CE3	2.56	0.41
1:O:153:ARG:HD3	1:O:205:THR:HG23	2.02	0.41
1:J:134:PHE:O	1:J:138:VAL:HG23	2.20	0.41
1:P:196:ILE:HD13	1:P:202:THR:HB	2.01	0.41
1:E:329:SER:HB2	1:E:377:VAL:HG13	2.02	0.41
1:A:178:ASP:HA	1:A:179:PRO:HD3	1.94	0.41
1:F:158:PRO:HB3	1:F:198:PRO:O	2.20	0.41
1:A:162:THR:HG23	1:E:162:THR:HG21	2.01	0.41
1:P:301:PRO:HD3	1:P:349:VAL:HG22	2.02	0.41
1:N:294:LEU:HD12	1:N:294:LEU:HA	1.80	0.41
1:D:105:LEU:HD12	1:D:246:ILE:HD11	2.02	0.41
1:A:159:LEU:HD13	1:N:167:ARG:NH2	2.35	0.41
1:P:114:ARG:HD2	1:P:181:PRO:HD2	2.02	0.41
1:M:271:SER:HB3	1:M:363:ASN:H	1.86	0.41
1:P:310:PHE:CE1	1:P:339:SER:HB2	2.55	0.41
1:D:310:PHE:CE1	1:D:339:SER:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:TRP:NE1	1:F:308:ILE:HD13	2.35	0.41
1:F:136:TRP:CZ2	1:H:143:ASN:HB3	2.55	0.41
1:P:60:ILE:HG21	1:P:60:ILE:HD13	1.49	0.41
1:P:203:LYS:HE2	1:P:203:LYS:HB3	1.81	0.41
1:D:225:LEU:HA	1:D:225:LEU:HD23	1.82	0.41
1:H:187:LEU:HD22	1:H:187:LEU:O	2.21	0.41
1:J:142:ALA:HB2	1:J:263:LEU:HD21	2.02	0.41
1:D:264:LEU:HB2	1:D:369:VAL:HG12	2.02	0.41
1:B:312:SER:HB2	1:B:313:THR:H	1.67	0.41
1:L:173:ASP:OD1	1:L:174:LYS:N	2.54	0.41
1:O:269:ARG:HE	1:O:289:ALA:HB3	1.86	0.41
1:K:121:ASN:HB3	1:K:123:ASP:H	1.86	0.41
1:A:292:THR:O	1:A:358:LEU:HB2	2.20	0.41
1:I:267:LEU:O	1:I:365:GLN:HA	2.21	0.41
1:H:188:ALA:HA	1:H:193:LEU:HD22	2.02	0.41
1:I:263:LEU:HA	1:I:263:LEU:HD23	1.93	0.41
1:I:284:PHE:CE1	1:I:298:ALA:HB2	2.55	0.41
1:B:335:THR:HG1	1:B:336:ALA:H	1.60	0.41
1:N:349:VAL:O	1:N:351:ALA:N	2.54	0.41
1:J:95:ARG:HG3	1:J:253:ASP:OD1	2.21	0.41
1:G:196:ILE:HG21	1:G:202:THR:HB	2.03	0.41
1:B:296:TRP:CD2	1:B:366:LEU:HD12	2.55	0.41
1:B:312:SER:O	1:B:337:GLY:HA2	2.21	0.41
1:I:169:ALA:CB	1:I:195:GLU:HG2	2.51	0.41
1:E:293:ASP:OD2	1:E:356:SER:HB2	2.21	0.41
1:I:318:THR:HG1	1:I:357:GLY:H	1.60	0.41
1:L:161:ASN:O	1:L:199:TRP:HB3	2.21	0.41
1:I:288:VAL:HG12	1:I:295:VAL:CG2	2.51	0.41
1:O:124:PHE:HE1	1:O:233:TRP:CH2	2.38	0.41
1:O:103:SER:HB2	1:O:132:PHE:CZ	2.56	0.41
1:L:224:LYS:HB3	1:M:214:PHE:CE2	2.55	0.41
1:F:271:SER:HA	1:F:272:ALA:HA	1.80	0.41
1:F:369:VAL:HG11	1:H:264:LEU:HD13	2.01	0.41
1:I:321:ILE:HA	1:I:352:ASN:O	2.21	0.41
1:I:312:SER:O	1:I:337:GLY:HA2	2.20	0.41
1:K:167:ARG:NH2	1:N:159:LEU:HD13	2.36	0.41
1:A:256:GLU:OE1	1:D:192:HIS:NE2	2.52	0.41
1:A:169:ALA:HA	1:A:194:SER:O	2.21	0.41
1:L:112:PHE:HE1	1:L:184:ARG:HG2	1.86	0.41
1:F:312:SER:O	1:F:337:GLY:HA2	2.20	0.41
1:A:159:LEU:HD12	1:A:159:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:PHE:HE1	1:L:233:TRP:CH2	2.39	0.40
1:E:291:ALA:HB1	1:E:360:GLY:HA2	2.04	0.40
1:H:291:ALA:HB1	1:H:360:GLY:HA2	2.03	0.40
1:H:294:LEU:HD12	1:H:294:LEU:HA	1.74	0.40
1:O:109:ASN:N	1:O:240:THR:HB	2.30	0.40
1:L:296:TRP:CD2	1:L:366:LEU:HD12	2.56	0.40
1:A:167:ARG:NH2	1:E:159:LEU:HD13	2.37	0.40
1:O:129:LEU:O	1:O:131:PRO:HD3	2.22	0.40
1:K:291:ALA:HB1	1:K:360:GLY:HA2	2.02	0.40
1:I:158:PRO:HB3	1:I:198:PRO:O	2.20	0.40
1:H:162:THR:HG23	1:K:162:THR:HG21	2.04	0.40
1:P:281:LEU:HD12	1:P:283:TYR:OH	2.22	0.40
1:D:314:VAL:N	1:D:336:ALA:O	2.44	0.40
1:E:167:ARG:HD2	1:E:195:GLU:HB3	2.02	0.40
1:J:95:ARG:NH2	1:J:150:ASN:ND2	2.69	0.40
1:M:264:LEU:HB2	1:M:369:VAL:HG12	2.03	0.40
1:L:267:LEU:O	1:L:365:GLN:HA	2.21	0.40
1:F:265:GLU:O	1:F:367:PHE:HA	2.21	0.40
1:N:335:THR:OG1	1:N:336:ALA:N	2.53	0.40
1:E:201:ILE:HG12	1:E:201:ILE:H	1.72	0.40
1:F:161:ASN:CB	1:J:165:ASN:HB3	2.48	0.40
1:M:105:LEU:HD12	1:M:246:ILE:HD11	2.02	0.40
1:F:113:LEU:HD12	1:F:113:LEU:HA	1.77	0.40
1:J:263:LEU:HD22	1:J:281:LEU:HD11	2.04	0.40
1:E:169:ALA:HA	1:E:194:SER:O	2.20	0.40
1:O:112:PHE:HE1	1:O:184:ARG:HG2	1.87	0.40
1:L:109:ASN:N	1:L:240:THR:HB	2.32	0.40
1:B:318:THR:CB	1:B:356:SER:HB2	2.48	0.40
1:G:272:ALA:O	1:G:274:SER:N	2.55	0.40
1:I:129:LEU:HD13	1:I:129:LEU:O	2.22	0.40
1:N:310:PHE:CE1	1:N:339:SER:HB2	2.57	0.40
1:O:149:PHE:CD1	1:O:252:VAL:HG13	2.57	0.40
1:G:162:THR:HA	1:G:199:TRP:CG	2.56	0.40
1:A:370:ARG:HA	1:A:370:ARG:HD3	1.63	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	288/380 (76%)	264 (92%)	17 (6%)	7 (2%)	7	27
1	B	290/380 (76%)	250 (86%)	24 (8%)	16 (6%)	2	6
1	D	321/380 (84%)	286 (89%)	25 (8%)	10 (3%)	5	19
1	E	288/380 (76%)	268 (93%)	13 (4%)	7 (2%)	7	27
1	F	290/380 (76%)	249 (86%)	25 (9%)	16 (6%)	2	6
1	G	321/380 (84%)	286 (89%)	25 (8%)	10 (3%)	5	19
1	H	288/380 (76%)	264 (92%)	17 (6%)	7 (2%)	7	27
1	I	290/380 (76%)	248 (86%)	26 (9%)	16 (6%)	2	6
1	J	321/380 (84%)	287 (89%)	24 (8%)	10 (3%)	5	19
1	K	288/380 (76%)	265 (92%)	16 (6%)	7 (2%)	7	27
1	L	290/380 (76%)	249 (86%)	23 (8%)	18 (6%)	2	5
1	M	321/380 (84%)	286 (89%)	24 (8%)	11 (3%)	5	17
1	N	288/380 (76%)	264 (92%)	17 (6%)	7 (2%)	7	27
1	O	290/380 (76%)	249 (86%)	25 (9%)	16 (6%)	2	6
1	P	321/380 (84%)	284 (88%)	28 (9%)	9 (3%)	6	22
All	All	4495/5700 (79%)	3999 (89%)	329 (7%)	167 (4%)	4	15

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	128	PRO
1	B	273	SER
1	B	314	VAL
1	B	317	LEU
1	B	350	ASN
1	D	118	THR
1	D	128	PRO
1	D	314	VAL

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Mol	Chain	Res	Type
1	F	128	PRO
1	F	273	SER
1	F	314	VAL
1	F	317	LEU
1	F	350	ASN
1	G	118	THR
1	G	128	PRO
1	G	314	VAL
1	I	128	PRO
1	I	273	SER
1	I	314	VAL
1	I	317	LEU
1	I	350	ASN
1	J	118	THR
1	J	128	PRO
1	J	314	VAL
1	L	128	PRO
1	L	273	SER
1	L	314	VAL
1	L	317	LEU
1	L	350	ASN
1	M	118	THR
1	M	128	PRO
1	M	314	VAL
1	O	128	PRO
1	O	273	SER
1	O	314	VAL
1	O	317	LEU
1	O	350	ASN
1	P	118	THR
1	P	128	PRO
1	P	314	VAL
1	A	273	SER
1	A	350	ASN
1	B	121	ASN
1	B	219	SER
1	B	336	ALA
1	B	337	GLY
1	B	349	VAL
1	D	117	GLY
1	E	273	SER
1	E	350	ASN

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Mol	Chain	Res	Type
1	F	121	ASN
1	F	219	SER
1	F	327	ILE
1	F	336	ALA
1	F	337	GLY
1	F	349	VAL
1	G	117	GLY
1	G	273	SER
1	H	273	SER
1	H	350	ASN
1	I	121	ASN
1	I	219	SER
1	I	336	ALA
1	I	337	GLY
1	I	349	VAL
1	J	117	GLY
1	K	273	SER
1	K	350	ASN
1	L	121	ASN
1	L	129	LEU
1	L	219	SER
1	L	327	ILE
1	L	336	ALA
1	L	337	GLY
1	L	349	VAL
1	N	273	SER
1	N	350	ASN
1	O	121	ASN
1	O	219	SER
1	O	336	ALA
1	O	337	GLY
1	O	349	VAL
1	B	120	PRO
1	B	338	SER
1	D	336	ALA
1	D	363	ASN
1	F	120	PRO
1	F	338	SER
1	G	274	SER
1	G	289	ALA
1	G	336	ALA
1	I	120	PRO

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Mol	Chain	Res	Type
1	I	338	SER
1	J	336	ALA
1	J	363	ASN
1	L	120	PRO
1	L	338	SER
1	M	117	GLY
1	M	336	ALA
1	O	120	PRO
1	O	327	ILE
1	O	338	SER
1	P	117	GLY
1	P	273	SER
1	P	336	ALA
1	P	363	ASN
1	B	327	ILE
1	D	273	SER
1	G	363	ASN
1	I	327	ILE
1	J	273	SER
1	M	61	ALA
1	M	273	SER
1	M	289	ALA
1	M	363	ASN
1	N	256	GLU
1	A	120	PRO
1	A	256	GLU
1	A	314	VAL
1	B	351	ALA
1	E	120	PRO
1	E	256	GLU
1	H	120	PRO
1	H	256	GLU
1	H	314	VAL
1	I	290	SER
1	I	351	ALA
1	J	61	ALA
1	J	91	LYS
1	K	120	PRO
1	K	256	GLU
1	L	290	SER
1	L	351	ALA
1	M	165	ASN

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Mol	Chain	Res	Type
1	M	256	GLU
1	N	120	PRO
1	O	290	SER
1	O	351	ALA
1	P	289	ALA
1	B	290	SER
1	D	91	LYS
1	D	256	GLU
1	D	289	ALA
1	F	290	SER
1	F	351	ALA
1	G	256	GLU
1	H	324	GLY
1	I	372	ILE
1	J	289	ALA
1	L	372	ILE
1	N	314	VAL
1	N	324	GLY
1	O	372	ILE
1	B	372	ILE
1	E	238	GLY
1	F	372	ILE
1	K	314	VAL
1	A	324	GLY
1	E	314	VAL
1	E	324	GLY
1	K	324	GLY
1	N	238	GLY
1	A	238	GLY
1	H	238	GLY
1	L	102	VAL
1	P	238	GLY
1	K	238	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/309 (79%)	210 (86%)	34 (14%)	4	11
1	B	245/309 (79%)	209 (85%)	36 (15%)	4	10
1	D	267/309 (86%)	232 (87%)	35 (13%)	5	13
1	E	244/309 (79%)	212 (87%)	32 (13%)	5	13
1	F	245/309 (79%)	208 (85%)	37 (15%)	3	9
1	G	267/309 (86%)	231 (86%)	36 (14%)	5	12
1	H	244/309 (79%)	213 (87%)	31 (13%)	5	15
1	I	245/309 (79%)	206 (84%)	39 (16%)	3	8
1	J	267/309 (86%)	230 (86%)	37 (14%)	4	11
1	K	244/309 (79%)	212 (87%)	32 (13%)	5	13
1	L	245/309 (79%)	207 (84%)	38 (16%)	3	9
1	M	267/309 (86%)	233 (87%)	34 (13%)	5	15
1	N	244/309 (79%)	210 (86%)	34 (14%)	4	11
1	O	245/309 (79%)	209 (85%)	36 (15%)	4	10
1	P	267/309 (86%)	232 (87%)	35 (13%)	5	13
All	All	3780/4635 (82%)	3254 (86%)	526 (14%)	4	11

All (526) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	A	99[A]	ARG
1	A	99[B]	ARG
1	A	103	SER
1	A	111	GLU
1	A	114	ARG
1	A	129	LEU
1	A	159	LEU
1	A	160	VAL
1	A	168	VAL
1	A	187	LEU
1	A	196	ILE
1	A	206	VAL
1	A	208	THR
1	A	211	VAL
1	A	228	LEU
1	A	252	VAL
1	A	266	SER

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Mol	Chain	Res	Type
1	A	292	THR
1	A	293	ASP
1	A	295	VAL
1	A	296	TRP
1	A	306	VAL
1	A	314	VAL
1	A	318	THR
1	A	327	ILE
1	A	333	VAL
1	A	335	THR
1	A	348	ARG
1	A	353	LEU
1	A	356	SER
1	A	374	GLU
1	A	377	VAL
1	A	380	VAL
1	B	93	SER
1	B	129	LEU
1	B	159	LEU
1	B	160	VAL
1	B	174	LYS
1	B	178	ASP
1	B	183	ASP
1	B	187	LEU
1	B	205	THR
1	B	225	LEU
1	B	228	LEU
1	B	252	VAL
1	B	264	LEU
1	B	266	SER
1	B	273	SER
1	B	288	VAL
1	B	292	THR
1	B	293	ASP
1	B	295	VAL
1	B	314	VAL
1	B	317	LEU
1	B	318	THR
1	B	327	ILE
1	B	330	SER
1	B	334	SER
1	B	335	THR

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Mol	Chain	Res	Type
1	B	342	VAL
1	B	348	ARG
1	B	349	VAL
1	B	352	ASN
1	B	359	THR
1	B	372	ILE
1	B	374	GLU
1	B	377	VAL
1	B	379	VAL
1	B	380	VAL
1	D	60	ILE
1	D	70	ILE
1	D	80	VAL
1	D	91	LYS
1	D	95	ARG
1	D	104	VAL
1	D	106	SER
1	D	129	LEU
1	D	133	LEU
1	D	139	ASN
1	D	145	ASP
1	D	151	SER
1	D	159	LEU
1	D	160	VAL
1	D	167	ARG
1	D	174	LYS
1	D	187	LEU
1	D	211	VAL
1	D	213	ARG
1	D	218	THR
1	D	225	LEU
1	D	237	SER
1	D	252	VAL
1	D	269	ARG
1	D	271	SER
1	D	275	VAL
1	D	317	LEU
1	D	329	SER
1	D	330	SER
1	D	333	VAL
1	D	349	VAL
1	D	359	THR

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Mol	Chain	Res	Type
1	D	373	THR
1	D	377	VAL
1	D	380	VAL
1	E	94	VAL
1	E	99[A]	ARG
1	E	99[B]	ARG
1	E	103	SER
1	E	111	GLU
1	E	114	ARG
1	E	129	LEU
1	E	159	LEU
1	E	160	VAL
1	E	168	VAL
1	E	187	LEU
1	E	196	ILE
1	E	206	VAL
1	E	208	THR
1	E	211	VAL
1	E	228	LEU
1	E	252	VAL
1	E	266	SER
1	E	292	THR
1	E	293	ASP
1	E	295	VAL
1	E	306	VAL
1	E	314	VAL
1	E	318	THR
1	E	327	ILE
1	E	333	VAL
1	E	335	THR
1	E	348	ARG
1	E	353	LEU
1	E	374	GLU
1	E	377	VAL
1	E	380	VAL
1	F	91	LYS
1	F	93	SER
1	F	129	LEU
1	F	159	LEU
1	F	160	VAL
1	F	174	LYS
1	F	178	ASP

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Mol	Chain	Res	Type
1	F	183	ASP
1	F	187	LEU
1	F	205	THR
1	F	206	VAL
1	F	225	LEU
1	F	228	LEU
1	F	252	VAL
1	F	266	SER
1	F	273	SER
1	F	288	VAL
1	F	292	THR
1	F	293	ASP
1	F	295	VAL
1	F	314	VAL
1	F	317	LEU
1	F	318	THR
1	F	327	ILE
1	F	330	SER
1	F	334	SER
1	F	335	THR
1	F	342	VAL
1	F	348	ARG
1	F	349	VAL
1	F	352	ASN
1	F	358	LEU
1	F	359	THR
1	F	372	ILE
1	F	374	GLU
1	F	379	VAL
1	F	380	VAL
1	G	70	ILE
1	G	80	VAL
1	G	83	ARG
1	G	91	LYS
1	G	95	ARG
1	G	106	SER
1	G	118	THR
1	G	129	LEU
1	G	133	LEU
1	G	139	ASN
1	G	145	ASP
1	G	151	SER

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Mol	Chain	Res	Type
1	G	159	LEU
1	G	160	VAL
1	G	167	ARG
1	G	174	LYS
1	G	187	LEU
1	G	211	VAL
1	G	213	ARG
1	G	218	THR
1	G	225	LEU
1	G	237	SER
1	G	252	VAL
1	G	269	ARG
1	G	271	SER
1	G	274	SER
1	G	275	VAL
1	G	317	LEU
1	G	329	SER
1	G	330	SER
1	G	333	VAL
1	G	349	VAL
1	G	359	THR
1	G	373	THR
1	G	377	VAL
1	G	380	VAL
1	H	94	VAL
1	H	99[A]	ARG
1	H	99[B]	ARG
1	H	103	SER
1	H	111	GLU
1	H	114	ARG
1	H	129	LEU
1	H	159	LEU
1	H	160	VAL
1	H	168	VAL
1	H	187	LEU
1	H	206	VAL
1	H	208	THR
1	H	211	VAL
1	H	228	LEU
1	H	252	VAL
1	H	266	SER
1	H	292	THR

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Mol	Chain	Res	Type
1	H	293	ASP
1	H	295	VAL
1	H	306	VAL
1	H	314	VAL
1	H	318	THR
1	H	327	ILE
1	H	333	VAL
1	H	335	THR
1	H	348	ARG
1	H	353	LEU
1	H	374	GLU
1	H	377	VAL
1	H	380	VAL
1	I	91	LYS
1	I	93	SER
1	I	129	LEU
1	I	159	LEU
1	I	160	VAL
1	I	174	LYS
1	I	178	ASP
1	I	183	ASP
1	I	187	LEU
1	I	205	THR
1	I	206	VAL
1	I	225	LEU
1	I	228	LEU
1	I	252	VAL
1	I	264	LEU
1	I	266	SER
1	I	273	SER
1	I	288	VAL
1	I	292	THR
1	I	293	ASP
1	I	295	VAL
1	I	314	VAL
1	I	317	LEU
1	I	318	THR
1	I	327	ILE
1	I	330	SER
1	I	334	SER
1	I	335	THR
1	I	342	VAL

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Mol	Chain	Res	Type
1	I	348	ARG
1	I	349	VAL
1	I	352	ASN
1	I	358	LEU
1	I	359	THR
1	I	372	ILE
1	I	374	GLU
1	I	377	VAL
1	I	379	VAL
1	I	380	VAL
1	J	70	ILE
1	J	80	VAL
1	J	83	ARG
1	J	91	LYS
1	J	95	ARG
1	J	106	SER
1	J	122	ASN
1	J	129	LEU
1	J	133	LEU
1	J	139	ASN
1	J	145	ASP
1	J	151	SER
1	J	159	LEU
1	J	160	VAL
1	J	167	ARG
1	J	174	LYS
1	J	187	LEU
1	J	210	ASN
1	J	211	VAL
1	J	213	ARG
1	J	218	THR
1	J	225	LEU
1	J	237	SER
1	J	252	VAL
1	J	269	ARG
1	J	271	SER
1	J	275	VAL
1	J	314	VAL
1	J	317	LEU
1	J	329	SER
1	J	330	SER
1	J	333	VAL

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Mol	Chain	Res	Type
1	J	349	VAL
1	J	359	THR
1	J	373	THR
1	J	377	VAL
1	J	380	VAL
1	K	94	VAL
1	K	99[A]	ARG
1	K	99[B]	ARG
1	K	103	SER
1	K	111	GLU
1	K	114	ARG
1	K	129	LEU
1	K	159	LEU
1	K	160	VAL
1	K	168	VAL
1	K	187	LEU
1	K	196	ILE
1	K	206	VAL
1	K	208	THR
1	K	211	VAL
1	K	228	LEU
1	K	252	VAL
1	K	266	SER
1	K	292	THR
1	K	293	ASP
1	K	296	TRP
1	K	306	VAL
1	K	314	VAL
1	K	318	THR
1	K	327	ILE
1	K	333	VAL
1	K	335	THR
1	K	348	ARG
1	K	353	LEU
1	K	374	GLU
1	K	377	VAL
1	K	380	VAL
1	L	93	SER
1	L	129	LEU
1	L	159	LEU
1	L	160	VAL
1	L	174	LYS

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Mol	Chain	Res	Type
1	L	178	ASP
1	L	183	ASP
1	L	187	LEU
1	L	205	THR
1	L	206	VAL
1	L	225	LEU
1	L	228	LEU
1	L	252	VAL
1	L	256	GLU
1	L	264	LEU
1	L	266	SER
1	L	273	SER
1	L	288	VAL
1	L	292	THR
1	L	293	ASP
1	L	295	VAL
1	L	314	VAL
1	L	317	LEU
1	L	318	THR
1	L	327	ILE
1	L	330	SER
1	L	334	SER
1	L	335	THR
1	L	342	VAL
1	L	348	ARG
1	L	349	VAL
1	L	352	ASN
1	L	359	THR
1	L	372	ILE
1	L	374	GLU
1	L	377	VAL
1	L	379	VAL
1	L	380	VAL
1	M	70	ILE
1	M	80	VAL
1	M	83	ARG
1	M	91	LYS
1	M	95	ARG
1	M	106	SER
1	M	129	LEU
1	M	133	LEU
1	M	139	ASN

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Mol	Chain	Res	Type
1	M	145	ASP
1	M	151	SER
1	M	159	LEU
1	M	160	VAL
1	M	167	ARG
1	M	174	LYS
1	M	187	LEU
1	M	211	VAL
1	M	213	ARG
1	M	218	THR
1	M	225	LEU
1	M	237	SER
1	M	252	VAL
1	M	269	ARG
1	M	271	SER
1	M	275	VAL
1	M	317	LEU
1	M	329	SER
1	M	330	SER
1	M	333	VAL
1	M	349	VAL
1	M	359	THR
1	M	373	THR
1	M	377	VAL
1	M	380	VAL
1	N	94	VAL
1	N	99[A]	ARG
1	N	99[B]	ARG
1	N	103	SER
1	N	111	GLU
1	N	114	ARG
1	N	129	LEU
1	N	159	LEU
1	N	160	VAL
1	N	168	VAL
1	N	187	LEU
1	N	196	ILE
1	N	201	ILE
1	N	206	VAL
1	N	208	THR
1	N	211	VAL
1	N	228	LEU

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Mol	Chain	Res	Type
1	N	252	VAL
1	N	266	SER
1	N	292	THR
1	N	293	ASP
1	N	295	VAL
1	N	296	TRP
1	N	306	VAL
1	N	314	VAL
1	N	318	THR
1	N	327	ILE
1	N	333	VAL
1	N	335	THR
1	N	348	ARG
1	N	353	LEU
1	N	374	GLU
1	N	377	VAL
1	N	380	VAL
1	O	93	SER
1	O	129	LEU
1	O	159	LEU
1	O	160	VAL
1	O	174	LYS
1	O	178	ASP
1	O	183	ASP
1	O	187	LEU
1	O	205	THR
1	O	206	VAL
1	O	225	LEU
1	O	228	LEU
1	O	252	VAL
1	O	266	SER
1	O	273	SER
1	O	288	VAL
1	O	292	THR
1	O	293	ASP
1	O	295	VAL
1	O	314	VAL
1	O	317	LEU
1	O	318	THR
1	O	327	ILE
1	O	330	SER
1	O	334	SER

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Mol	Chain	Res	Type
1	O	335	THR
1	O	342	VAL
1	O	348	ARG
1	O	349	VAL
1	O	352	ASN
1	O	359	THR
1	O	372	ILE
1	O	374	GLU
1	O	377	VAL
1	O	379	VAL
1	O	380	VAL
1	P	60	ILE
1	P	70	ILE
1	P	80	VAL
1	P	83	ARG
1	P	91	LYS
1	P	95	ARG
1	P	106	SER
1	P	129	LEU
1	P	133	LEU
1	P	139	ASN
1	P	145	ASP
1	P	151	SER
1	P	159	LEU
1	P	160	VAL
1	P	167	ARG
1	P	174	LYS
1	P	187	LEU
1	P	211	VAL
1	P	213	ARG
1	P	218	THR
1	P	225	LEU
1	P	237	SER
1	P	252	VAL
1	P	269	ARG
1	P	271	SER
1	P	275	VAL
1	P	317	LEU
1	P	329	SER
1	P	330	SER
1	P	333	VAL
1	P	349	VAL

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Mol	Chain	Res	Type
1	P	359	THR
1	P	373	THR
1	P	377	VAL
1	P	380	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	B	122	ASN
1	D	150	ASN
1	D	165	ASN
1	D	328	ASN
1	F	122	ASN
1	F	297	GLN
1	G	150	ASN
1	G	328	ASN
1	I	122	ASN
1	J	150	ASN
1	J	328	ASN
1	K	363	ASN
1	M	150	ASN
1	M	328	ASN
1	N	363	ASN
1	O	122	ASN
1	O	297	GLN
1	P	150	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	289/380 (76%)	-0.01	9 (3%) 52 46	27, 46, 93, 118	0
1	B	291/380 (76%)	0.19	14 (4%) 34 29	27, 51, 102, 117	0
1	D	321/380 (84%)	-0.09	5 (1%) 74 73	28, 46, 91, 107	0
1	E	289/380 (76%)	0.01	5 (1%) 73 71	27, 46, 87, 110	0
1	F	291/380 (76%)	0.14	13 (4%) 37 31	25, 51, 107, 124	0
1	G	321/380 (84%)	-0.06	4 (1%) 81 79	26, 45, 87, 105	0
1	H	289/380 (76%)	0.05	12 (4%) 40 34	29, 46, 92, 103	0
1	I	291/380 (76%)	0.23	16 (5%) 29 23	27, 51, 104, 120	0
1	J	321/380 (84%)	-0.09	3 (0%) 85 84	29, 46, 87, 111	0
1	K	289/380 (76%)	0.01	8 (2%) 56 51	28, 47, 85, 111	0
1	L	291/380 (76%)	0.22	23 (7%) 15 10	29, 51, 105, 124	0
1	M	321/380 (84%)	-0.05	4 (1%) 81 79	28, 46, 85, 102	0
1	N	289/380 (76%)	-0.04	7 (2%) 62 58	28, 48, 89, 117	0
1	O	291/380 (76%)	0.22	20 (6%) 20 15	26, 52, 107, 125	0
1	P	321/380 (84%)	0.00	8 (2%) 61 57	26, 47, 93, 111	0
All	All	4505/5700 (79%)	0.05	151 (3%) 49 42	25, 47, 99, 125	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	272	ALA	5.8
1	F	272	ALA	5.4
1	L	90	ALA	5.3
1	I	121	ASN	5.0
1	A	314	VAL	4.9
1	I	272	ALA	4.8
1	J	314	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	M	314	VAL	4.3
1	M	122	ASN	4.1
1	D	314	VAL	3.9
1	L	312	SER	3.9
1	L	362	THR	3.9
1	O	271	SER	3.8
1	L	334	SER	3.7
1	O	272	ALA	3.7
1	G	91	LYS	3.6
1	N	314	VAL	3.5
1	O	312	SER	3.5
1	O	358	LEU	3.5
1	A	271	SER	3.4
1	B	271	SER	3.3
1	N	271	SER	3.2
1	L	272	ALA	3.2
1	O	121	ASN	3.2
1	M	356	SER	3.1
1	P	314	VAL	3.0
1	I	310	PHE	3.0
1	D	316	GLY	3.0
1	F	121	ASN	3.0
1	L	121	ASN	2.9
1	L	358	LEU	2.9
1	N	317	LEU	2.9
1	B	289	ALA	2.9
1	O	334	SER	2.9
1	H	335	THR	2.9
1	L	380	VAL	2.9
1	B	317	LEU	2.9
1	F	361	ALA	2.9
1	A	275	VAL	2.9
1	H	314	VAL	2.9
1	B	121	ASN	2.9
1	D	289	ALA	2.8
1	F	90	ALA	2.8
1	O	322	SER	2.8
1	G	314	VAL	2.8
1	P	273	SER	2.8
1	L	325	GLY	2.7
1	M	289	ALA	2.7
1	L	363	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	334	SER	2.7
1	K	358	LEU	2.7
1	I	337	GLY	2.7
1	B	315	GLY	2.6
1	F	289	ALA	2.6
1	I	92	GLY	2.6
1	B	310	PHE	2.6
1	O	353	LEU	2.6
1	I	275	VAL	2.6
1	B	349	VAL	2.6
1	B	362	THR	2.6
1	P	316	GLY	2.6
1	L	275	VAL	2.6
1	E	316	GLY	2.6
1	I	290	SER	2.6
1	K	334	SER	2.6
1	O	290	SER	2.6
1	O	337	GLY	2.6
1	I	288	VAL	2.6
1	O	314	VAL	2.6
1	G	122	ASN	2.5
1	F	314	VAL	2.5
1	L	314	VAL	2.5
1	A	317	LEU	2.5
1	B	90	ALA	2.4
1	I	271	SER	2.4
1	I	90	ALA	2.4
1	O	333	VAL	2.4
1	H	296	TRP	2.4
1	L	289	ALA	2.4
1	A	362	THR	2.4
1	I	312	SER	2.4
1	H	313	THR	2.4
1	F	317	LEU	2.4
1	F	315	GLY	2.4
1	H	274	SER	2.4
1	K	271	SER	2.4
1	F	271	SER	2.3
1	H	312	SER	2.3
1	I	349	VAL	2.3
1	I	289	ALA	2.3
1	H	271	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	324	GLY	2.3
1	P	272	ALA	2.3
1	I	294	LEU	2.3
1	L	361	ALA	2.3
1	K	270	GLU	2.3
1	O	92	GLY	2.3
1	J	122	ASN	2.3
1	N	363	ASN	2.3
1	G	218	THR	2.3
1	H	355	LEU	2.3
1	E	335	THR	2.2
1	I	317	LEU	2.2
1	O	362	THR	2.2
1	F	358	LEU	2.2
1	P	359	THR	2.2
1	H	334	SER	2.2
1	L	337	GLY	2.2
1	O	317	LEU	2.2
1	P	91	LYS	2.2
1	E	270	GLU	2.2
1	F	312	SER	2.2
1	L	91	LYS	2.2
1	O	275	VAL	2.2
1	O	349	VAL	2.2
1	N	313	THR	2.2
1	B	312	SER	2.2
1	O	289	ALA	2.2
1	O	315	GLY	2.2
1	K	315	GLY	2.1
1	A	270	GLU	2.1
1	K	316	GLY	2.1
1	D	221	GLY	2.1
1	N	120	PRO	2.1
1	H	359	THR	2.1
1	K	335	THR	2.1
1	A	361	ALA	2.1
1	A	337	GLY	2.1
1	F	91	LYS	2.1
1	P	221	GLY	2.1
1	E	273	SER	2.1
1	F	334	SER	2.1
1	L	351	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	315	GLY	2.1
1	L	359	THR	2.1
1	D	91	LYS	2.1
1	L	320	SER	2.1
1	H	319	PRO	2.1
1	B	269	ARG	2.1
1	L	290	SER	2.0
1	O	355	LEU	2.0
1	L	364	ALA	2.0
1	L	315	GLY	2.0
1	N	358	LEU	2.0
1	B	92	GLY	2.0
1	P	220	SER	2.0
1	H	358	LEU	2.0
1	K	317	LEU	2.0
1	L	355	LEU	2.0
1	J	340	ALA	2.0
1	E	271	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	CA	B	401	1/1	0.91	0.37	17.34	89,89,89,89	0
2	CA	O	402	1/1	0.82	0.28	4.48	87,87,87,87	0
2	CA	K	402	1/1	0.78	0.23	4.38	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	N	401	1/1	0.66	0.20	2.84	88,88,88,88	0
2	CA	E	402	1/1	0.92	0.22	2.28	93,93,93,93	0
3	ZN	J	401[A]	1/1	0.79	0.21	0.34	97,97,97,97	1
2	CA	I	401	1/1	0.74	0.17	0.26	99,99,99,99	0
3	ZN	D	401[A]	1/1	0.79	0.21	0.18	97,97,97,97	1
3	ZN	P	401[B]	1/1	0.79	0.21	0.18	102,102,102,102	0
3	ZN	D	401[B]	1/1	0.79	0.21	-0.33	121,121,121,121	1
3	ZN	J	401[B]	1/1	0.79	0.21	-0.33	121,121,121,121	1
3	ZN	P	401[A]	1/1	0.79	0.21	-0.33	120,120,120,120	1
2	CA	F	401	1/1	0.84	0.14	-0.34	82,82,82,82	0
2	CA	D	402	1/1	0.95	0.13	-0.70	77,77,77,77	0
2	CA	I	402	1/1	0.78	0.12	-1.69	91,91,91,91	0
2	CA	K	401	1/1	0.89	0.10	-4.06	77,77,77,77	0
3	ZN	M	401[A]	1/1	0.91	0.23	-	107,107,107,107	1
2	CA	B	402	1/1	0.72	0.12	-	84,84,84,84	0
2	CA	M	402	1/1	0.86	0.12	-	74,74,74,74	0
2	CA	E	401	1/1	0.70	0.20	-	82,82,82,82	0
3	ZN	G	401[A]	1/1	0.86	0.21	-	99,99,99,99	1
3	ZN	M	401[B]	1/1	0.91	0.23	-	118,118,118,118	1
3	ZN	G	401[B]	1/1	0.86	0.21	-	124,124,124,124	1
2	CA	O	401	1/1	0.91	0.15	-	76,76,76,76	0
2	CA	H	401	1/1	0.93	0.12	-	77,77,77,77	0

6.5 Other polymers

There are no such residues in this entry.