



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:20 AM UTC

PDB ID : 5J7U / pdb_00005j7u
Title : Faustovirus major capsid protein
Authors : Klose, T.; Rossmann, M.G.
Deposited on : 2016-04-06
Resolution : 2.44 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

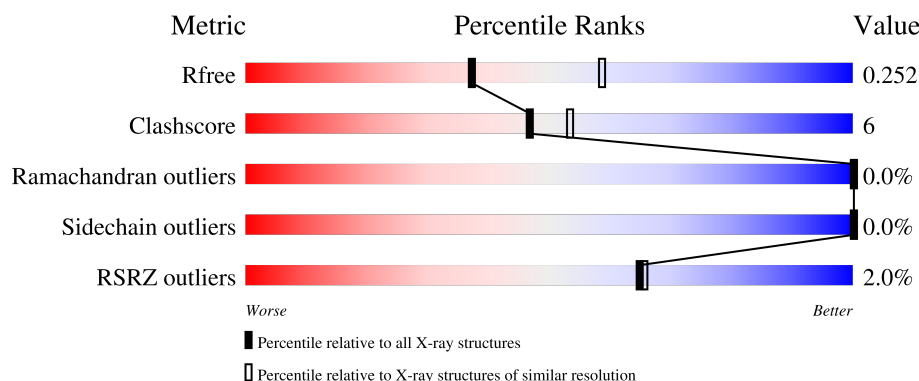
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	645	83% 12% 6%
1	B	645	82% 14% .
1	C	645	4% 81% 14% .
1	D	645	82% 12% 6%
1	E	645	4% 82% 13% .

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Mol	Chain	Length	Quality of chain
1	F	645	 2% 82% 12% 5%
1	G	645	 % 81% 13% 5%
1	H	645	 2% 85% 10% 5%
1	I	645	 3% 81% 15% 5%
1	J	645	 83% 11% 5%
1	K	645	 2% 81% 14% 5%
1	L	645	 2% 82% 12% 5%
2	M	21	 100%
2	N	21	 90% 10%
2	O	21	 100%
2	P	21	 95% 5%
2	Q	21	 76% 24%
2	R	21	 71% 19% 10%
2	S	21	 86% 14%
2	T	21	 100%
2	U	21	 95% 5%
2	V	21	 86% 14%
2	W	21	 90% 10%
2	X	21	 67% 24% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 61035 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 major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4785	3060	803	908	14			
1	B	616	Total	C	N	O	S	0	0	0
			4837	3092	812	919	14			
1	C	616	Total	C	N	O	S	0	0	0
			4842	3098	812	918	14			
1	D	609	Total	C	N	O	S	0	0	0
			4785	3060	803	908	14			
1	E	616	Total	C	N	O	S	0	0	0
			4841	3097	812	918	14			
1	F	610	Total	C	N	O	S	0	0	0
			4793	3064	804	911	14			
1	G	611	Total	C	N	O	S	0	0	0
			4799	3067	805	913	14			
1	H	615	Total	C	N	O	S	0	0	0
			4831	3089	811	917	14			
1	I	616	Total	C	N	O	S	0	0	0
			4842	3098	812	918	14			
1	J	610	Total	C	N	O	S	0	0	0
			4793	3064	804	911	14			
1	K	614	Total	C	N	O	S	0	0	0
			4823	3083	810	916	14			
1	L	610	Total	C	N	O	S	0	0	0
			4793	3064	804	911	14			

- Molecule 2 is a protein called unknown.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	N	21	Total	C	N	O	0	0	0
			105	63	21	21			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	P	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	Q	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	R	19	Total	C	N	O	0	0	0
			95	57	19	19			
2	S	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	T	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	U	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	V	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	W	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	X	19	Total	C	N	O	0	0	0
			95	57	19	19			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	173	Total	O	0	0
			173	173		
3	B	170	Total	O	0	0
			170	170		
3	C	164	Total	O	0	0
			164	164		
3	D	191	Total	O	0	0
			191	191		
3	E	168	Total	O	0	0
			168	168		
3	F	172	Total	O	0	0
			172	172		
3	N	2	Total	O	0	0
			2	2		
3	O	2	Total	O	0	0
			2	2		
3	P	5	Total	O	0	0
			5	5		

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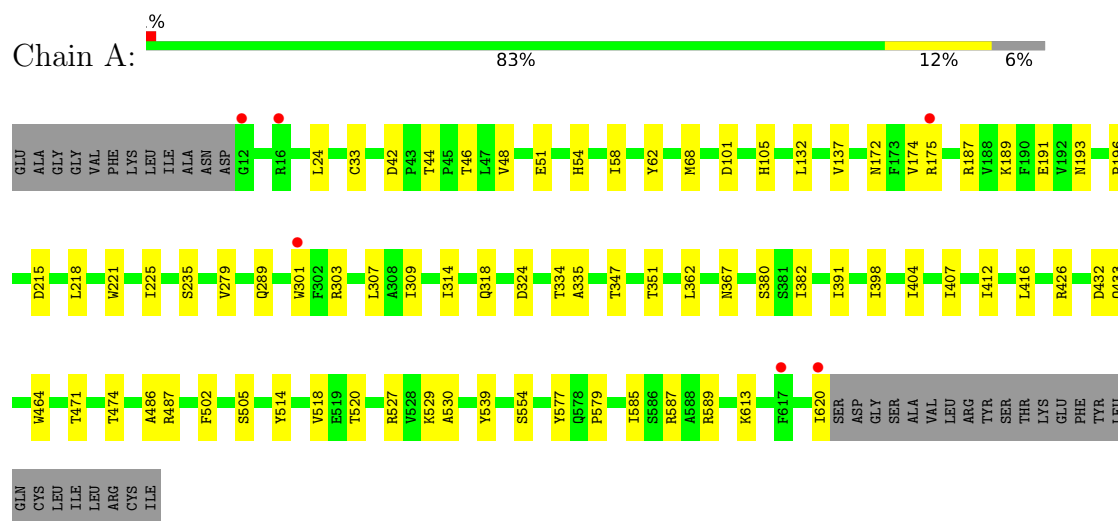
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Q	2	Total 2	O 2	0	0
3	R	2	Total 2	O 2	0	0
3	G	176	Total 176	O 176	0	0
3	H	165	Total 165	O 165	0	0
3	I	133	Total 133	O 133	0	0
3	J	163	Total 163	O 163	0	0
3	K	156	Total 156	O 156	0	0
3	L	171	Total 171	O 171	0	0
3	S	1	Total 1	O 1	0	0
3	U	7	Total 7	O 7	0	0
3	V	3	Total 3	O 3	0	0
3	W	2	Total 2	O 2	0	0
3	X	3	Total 3	O 3	0	0

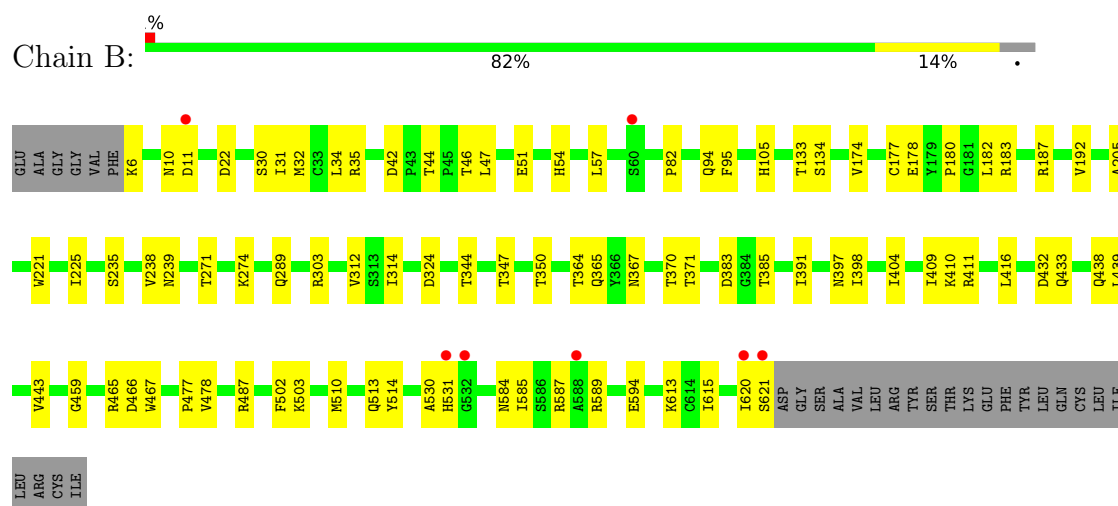
3 Residue-property plots [i](#)

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

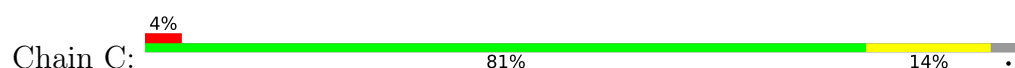
- Molecule 1: major capsid protein

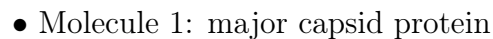


- Molecule 1: major capsid protein

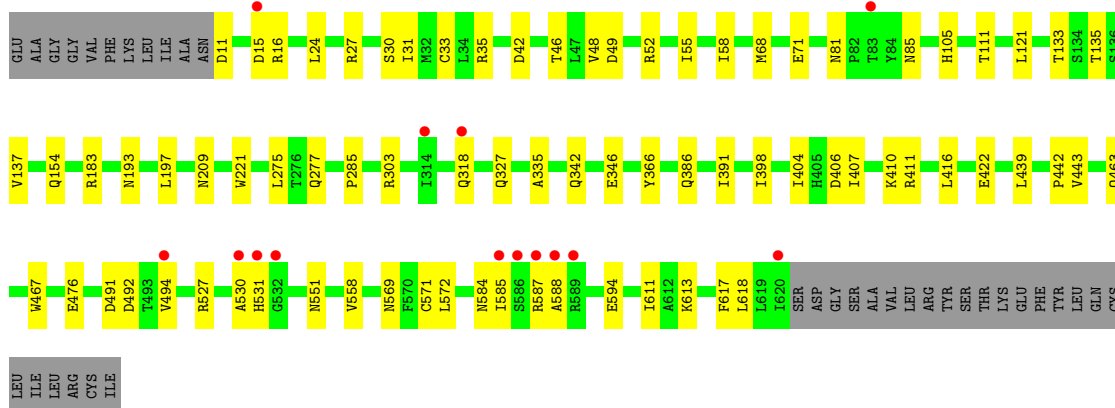


- Molecule 1: major capsid protein



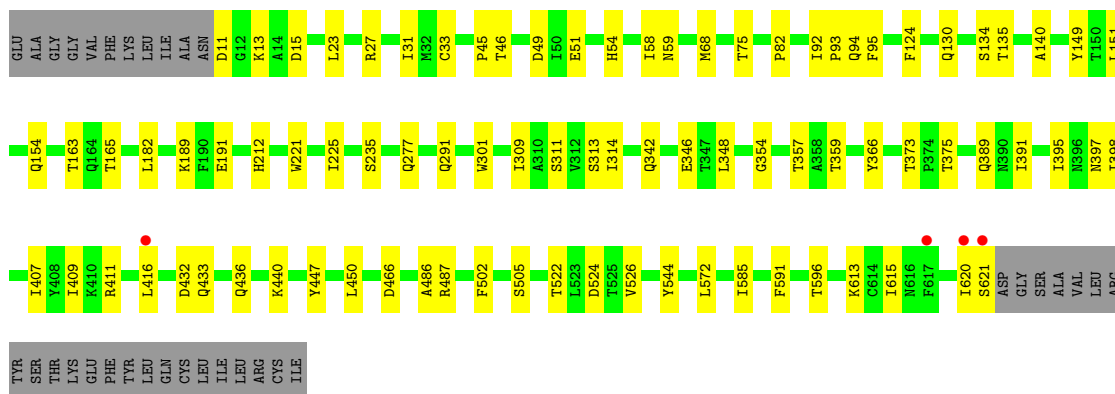


Chain F: 



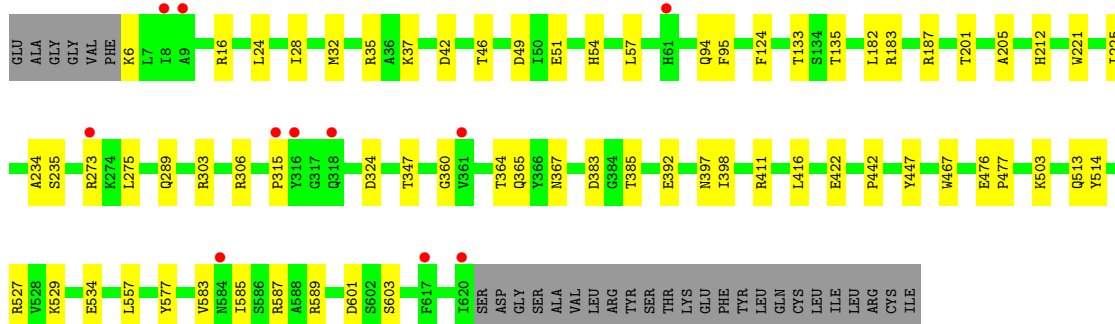
• Molecule 1: major capsid protein

Chain G: 



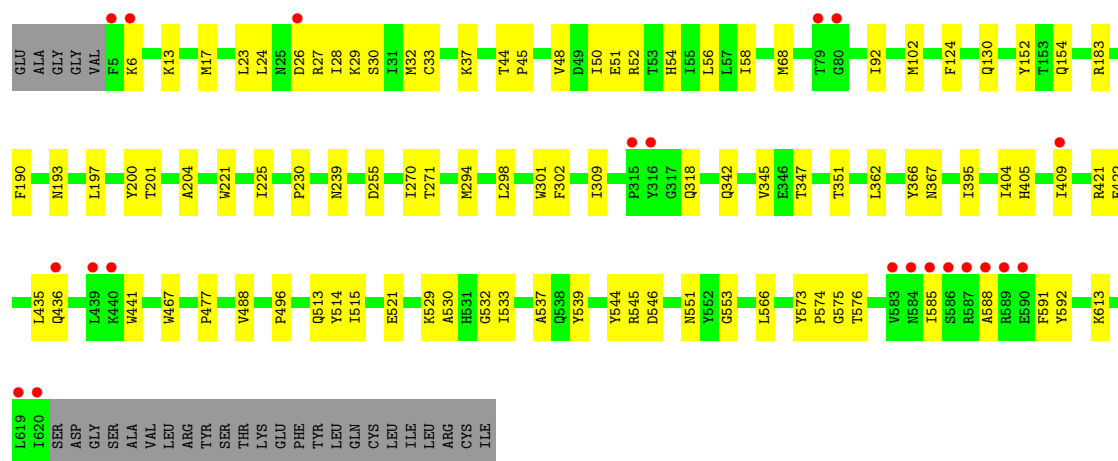
• Molecule 1: major capsid protein

Chain H: 



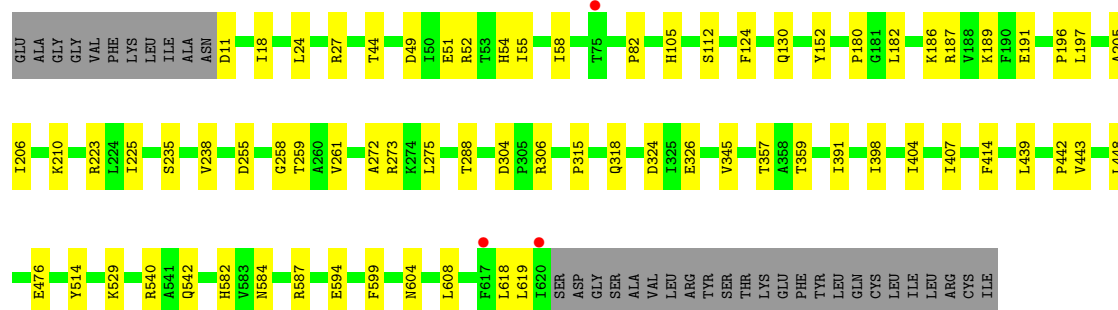
• Molecule 1: major capsid protein

Chain I: 



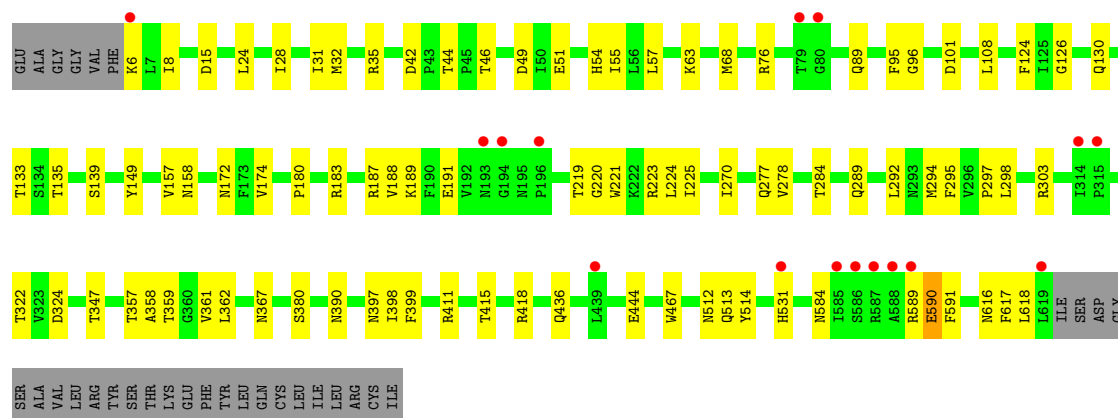
- Molecule 1: major capsid protein

Chain J: 83% 11% 5%



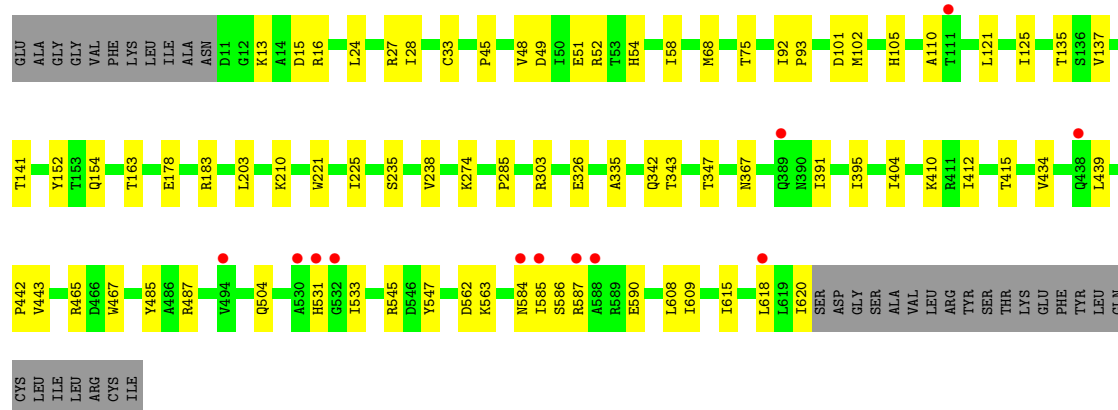
- Molecule 1: major capsid protein

Chain K: 81% 14% 5%



- Molecule 1: major capsid protein

Chain L: 82% 12% 5%



- Molecule 2: unknown

Chain M:  100%

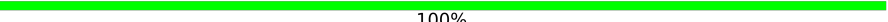
There are no outlier residues recorded for this chain.

- Molecule 2: unknown

Chain N:  90%  10%



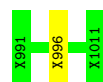
- Molecule 2: unknown

Chain O:  100%

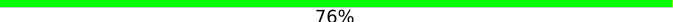
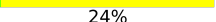
There are no outlier residues recorded for this chain.

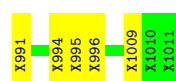
- Molecule 2: unknown

Chain P:  95%  5%

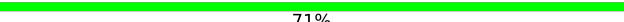
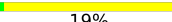


- Molecule 2: unknown

Chain Q:  76%  24%

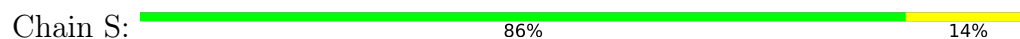


- Molecule 2: unknown

Chain R:  71%  19%  10%



- Molecule 2: unknown

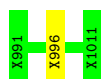


- Molecule 2: unknown

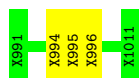
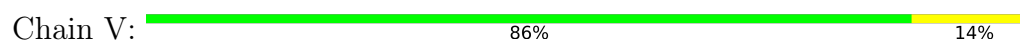


There are no outlier residues recorded for this chain.

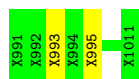
- Molecule 2: unknown



- Molecule 2: unknown



- Molecule 2: unknown



- Molecule 2: unknown



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.38Å 390.83Å 130.14Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	72.92 – 2.44 72.92 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.6 (72.92-2.44) 99.8 (72.92-2.44)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.205 , 0.252 0.205 , 0.252	Depositor DCC
R_{free} test set	15727 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	61035	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 46.29 % 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 1.1691e-04. 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](#)

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	0.13	0/4901	0.37	1/6697 (0.0%)
1	B	0.13	0/4953	0.37	0/6767
1	C	0.19	1/4959 (0.0%)	0.36	1/6775 (0.0%)
1	D	0.13	0/4901	0.34	0/6697
1	E	0.14	0/4958	0.36	0/6774
1	F	0.13	0/4909	0.35	0/6708
1	G	0.15	0/4915	0.37	0/6716
1	H	0.13	0/4947	0.34	0/6759
1	I	0.13	0/4959	0.37	0/6775
1	J	0.12	0/4909	0.36	1/6708 (0.0%)
1	K	0.15	0/4939	0.36	0/6748
1	L	0.15	0/4909	0.36	0/6708
All	All	0.14	1/59159 (0.0%)	0.36	3/80832 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	412	ILE	CB-CG1	-5.08	1.43	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	238	VAL	N-CA-C	-6.63	106.33	112.96
1	A	554	SER	CB-CA-C	-6.14	109.47	116.54
1	C	412	ILE	CB-CG1-CD1	-5.87	101.47	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4785	0	4711	78	0
1	B	4837	0	4766	66	0
1	C	4842	0	4770	66	0
1	D	4785	0	4711	65	0
1	E	4841	0	4768	75	0
1	F	4793	0	4715	58	0
1	G	4799	0	4720	57	0
1	H	4831	0	4761	50	0
1	I	4842	0	4770	66	0
1	J	4793	0	4715	56	0
1	K	4823	0	4750	66	0
1	L	4793	0	4715	56	0
2	M	105	0	24	0	0
2	N	105	0	24	2	0
2	O	105	0	24	0	0
2	P	105	0	24	1	0
2	Q	105	0	24	4	0
2	R	95	0	21	4	0
2	S	105	0	24	3	0
2	T	105	0	24	0	0
2	U	105	0	25	1	0
2	V	105	0	25	3	0
2	W	105	0	24	1	0
2	X	95	0	22	5	0
3	A	173	0	0	4	0
3	B	170	0	0	5	0
3	C	164	0	0	2	0
3	D	191	0	0	4	0
3	E	168	0	0	3	0
3	F	172	0	0	3	0
3	G	176	0	0	5	0
3	H	165	0	0	7	0
3	I	133	0	0	4	0
3	J	163	0	0	4	0
3	K	156	0	0	4	0
3	L	171	0	0	5	0
3	N	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	2	0	0	0	0
3	P	5	0	0	0	0
3	Q	2	0	0	1	0
3	R	2	0	0	2	0
3	S	1	0	0	1	0
3	U	7	0	0	0	0
3	V	3	0	0	0	0
3	W	2	0	0	1	0
3	X	3	0	0	4	0
All	All	61035	0	57157	660	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 6.

All (660) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ARG:HH12	1:A:529:LYS:CE	1.25	1.44
1:D:62:TYR:CE1	1:E:416:LEU:CD1	2.02	1.43
1:D:62:TYR:CE1	1:E:416:LEU:HD13	1.53	1.40
1:A:527:ARG:NH1	1:A:529:LYS:HE3	1.36	1.36
1:I:318:GLN:CD	3:I:701:HOH:O	1.73	1.30
1:A:351:THR:OG1	1:A:362:LEU:HD22	1.14	1.30
1:D:62:TYR:CZ	1:E:416:LEU:HD11	1.74	1.22
1:I:318:GLN:NE2	3:I:701:HOH:O	1.71	1.07
1:A:351:THR:OG1	1:A:362:LEU:CD2	2.02	1.07
1:D:62:TYR:CD1	1:E:416:LEU:HD13	1.97	0.99
1:D:62:TYR:CZ	1:E:416:LEU:CD1	2.42	0.91
1:A:527:ARG:HH12	1:A:529:LYS:HE3	0.74	0.91
1:C:436:GLN:HB3	1:C:439:LEU:HD23	1.50	0.91
1:D:404:ILE:HD11	1:F:24:LEU:HD21	1.54	0.88
1:D:273:ARG:HE	1:E:284:THR:HG22	1.37	0.87
1:A:527:ARG:NH1	1:A:529:LYS:CE	2.08	0.83
1:K:35:ARG:NH1	1:K:42:ASP:O	2.13	0.81
1:E:582:HIS:NE2	1:F:15:ASP:OD1	2.13	0.80
1:A:351:THR:HG1	1:A:362:LEU:HD22	0.99	0.80
1:D:62:TYR:HE1	1:E:416:LEU:CD1	1.90	0.80
1:F:35:ARG:NH2	1:F:42:ASP:O	2.17	0.77
1:D:44:THR:O	1:E:411:ARG:NH2	2.18	0.76
1:B:187:ARG:NH1	1:B:324:ASP:OD2	2.18	0.76
1:G:75:THR:HG21	1:G:93:PRO:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:273:ARG:HE	1:K:284:THR:HG22	1.51	0.75
1:E:500:THR:O	1:E:503:LYS:NZ	2.21	0.74
1:A:46:THR:HG22	1:A:48:VAL:H	1.52	0.74
1:J:112:SER:HB3	1:J:288:THR:HG22	1.69	0.73
1:B:433:GLN:HG2	1:B:594:GLU:HG2	1.70	0.73
1:D:62:TYR:OH	1:E:416:LEU:HD11	1.89	0.72
1:A:175:ARG:HH11	1:A:335:ALA:HB2	1.53	0.72
1:H:303:ARG:NH1	1:I:551:ASN:OD1	2.21	0.72
1:K:180:PRO:HB2	1:K:294:MET:HE1	1.70	0.72
1:A:527:ARG:HH12	1:A:529:LYS:CD	2.02	0.72
1:G:357:THR:HG23	1:G:359:THR:H	1.55	0.72
1:I:26:ASP:HA	1:I:29:LYS:HG2	1.71	0.72
1:D:58:ILE:HD11	1:E:398:ILE:HG21	1.72	0.72
1:J:540:ARG:NH1	1:J:542:GLN:OE1	2.24	0.71
1:F:133:THR:HG23	1:F:135:THR:H	1.56	0.71
1:B:178:GLU:HG3	1:B:465:ARG:HA	1.73	0.71
1:G:189:LYS:NZ	1:G:191:GLU:OE2	2.22	0.71
1:I:33:CYS:SG	3:I:793:HOH:O	2.48	0.70
1:G:13:LYS:NZ	2:S:1009:UNK:O	2.24	0.70
2:S:991:UNK:N	3:S:1101:HOH:O	2.25	0.70
1:A:527:ARG:HH12	1:A:529:LYS:HE2	1.50	0.70
1:F:16:ARG:NH2	3:F:705:HOH:O	2.25	0.69
1:H:35:ARG:NH2	1:H:42:ASP:O	2.25	0.69
1:B:585:ILE:HG22	1:B:589:ARG:HE	1.58	0.69
1:H:306:ARG:NH1	3:H:705:HOH:O	2.24	0.69
1:L:33:CYS:SG	3:L:834:HOH:O	2.49	0.69
1:K:357:THR:OG1	1:K:359:THR:HG22	1.93	0.68
1:D:35:ARG:NH2	1:D:42:ASP:O	2.23	0.68
1:K:133:THR:HG23	1:K:135:THR:H	1.57	0.68
1:F:81:ASN:OD1	1:F:81:ASN:O	2.11	0.68
1:E:357:THR:OG1	1:E:359:THR:HG22	1.92	0.68
1:J:58:ILE:HD11	1:K:398:ILE:HG21	1.75	0.68
1:G:613:LYS:NZ	3:G:703:HOH:O	2.26	0.68
1:E:31:ILE:HG21	1:E:45:PRO:HB3	1.76	0.68
1:I:102:MET:HE3	1:I:298:LEU:HD12	1.74	0.68
1:L:531:HIS:CD2	1:L:587:ARG:HA	2.29	0.68
1:E:44:THR:O	1:F:411:ARG:NH2	2.22	0.67
1:A:33:CYS:SG	3:A:850:HOH:O	2.51	0.67
1:A:539:TYR:HE1	1:C:74:LYS:HZ2	1.40	0.67
1:B:35:ARG:NH1	1:B:42:ASP:O	2.27	0.67
1:J:27:ARG:NH2	1:J:49:ASP:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:6:LYS:N	3:K:707:HOH:O	2.28	0.67
1:A:412:ILE:HG23	1:A:620:ILE:HG13	1.77	0.67
1:G:212:HIS:NE2	1:G:447:TYR:OH	2.23	0.66
1:A:58:ILE:HD11	1:B:398:ILE:HG21	1.77	0.66
1:A:351:THR:HG1	1:A:362:LEU:CD2	1.92	0.65
1:H:133:THR:HG22	1:H:135:THR:H	1.61	0.65
1:C:92:ILE:HD11	1:C:321:ILE:HG12	1.79	0.65
1:B:530:ALA:HB1	1:B:587:ARG:HB3	1.77	0.65
1:E:416:LEU:HB2	1:E:577:TYR:OH	1.95	0.65
1:B:6:LYS:N	3:B:713:HOH:O	2.30	0.65
1:F:33:CYS:SG	3:R:1102:HOH:O	2.54	0.65
1:G:11:ASP:N	1:G:15:ASP:OD2	2.29	0.65
1:I:521:GLU:OE2	1:I:545:ARG:NH2	2.30	0.65
1:G:46:THR:HG23	1:G:49:ASP:H	1.62	0.64
1:A:613:LYS:NZ	3:A:705:HOH:O	2.30	0.64
1:F:85:ASN:HB2	1:F:327:GLN:HG2	1.78	0.64
1:G:46:THR:HA	1:H:411:ARG:HD2	1.79	0.64
1:A:189:LYS:HE3	1:A:196:PRO:HG3	1.80	0.64
1:J:18:ILE:HD11	1:L:615:ILE:HG21	1.79	0.64
1:C:35:ARG:NH2	3:C:708:HOH:O	2.30	0.63
1:K:436:GLN:O	3:K:701:HOH:O	2.15	0.63
1:G:277:GLN:NE2	3:G:707:HOH:O	2.28	0.63
1:D:291:GLN:O	3:D:701:HOH:O	2.15	0.63
1:E:408:TYR:O	1:E:412:ILE:HG22	1.99	0.63
1:I:37:LYS:NZ	3:I:708:HOH:O	2.30	0.63
1:K:584:ASN:ND2	1:L:15:ASP:OD2	2.32	0.63
1:A:351:THR:CB	1:A:362:LEU:HD22	2.24	0.63
1:I:52:ARG:NH1	2:U:996:UNK:O	2.33	0.62
1:B:303:ARG:NH1	1:C:551:ASN:OD1	2.32	0.62
1:I:301:TRP:CH2	1:I:309:ILE:HD11	2.34	0.62
1:B:82:PRO:HG3	1:B:391:ILE:HG22	1.80	0.62
1:A:175:ARG:NH1	1:A:334:THR:O	2.29	0.62
1:A:398:ILE:HG21	1:C:58:ILE:HD11	1.81	0.62
1:A:527:ARG:HH22	1:A:529:LYS:HE2	1.64	0.62
1:E:94:GLN:OE1	1:E:311:SER:OG	2.13	0.62
1:F:197:LEU:HD21	1:F:618:LEU:HD21	1.79	0.62
1:E:440:LYS:HG3	1:E:441:TRP:CD1	2.35	0.62
1:A:530:ALA:HB1	1:A:587:ARG:HB3	1.82	0.62
1:G:313:SER:HA	1:G:621:SER:HB2	1.82	0.61
1:B:584:ASN:ND2	1:C:15:ASP:OD2	2.29	0.61
1:I:405:HIS:CE1	1:I:409:ILE:HD11	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:VAL:HG23	1:D:317:GLY:HA3	1.83	0.61
1:D:189:LYS:HD3	1:D:196:PRO:HB3	1.81	0.61
1:D:547:TYR:OH	1:F:303:ARG:NH2	2.34	0.60
1:A:426:ARG:NH2	3:A:709:HOH:O	2.34	0.60
1:D:47:LEU:HD22	1:D:56:LEU:HD11	1.83	0.60
1:A:187:ARG:NH1	1:A:324:ASP:OD2	2.32	0.60
1:B:10:ASN:ND2	1:B:22:ASP:OD2	2.34	0.60
1:J:11:ASP:OD2	1:L:584:ASN:ND2	2.33	0.60
1:E:362:LEU:HG	1:F:492:ASP:HB3	1.83	0.60
1:F:587:ARG:NH2	3:F:711:HOH:O	2.35	0.60
1:C:529:LYS:NZ	3:C:710:HOH:O	2.33	0.60
2:Q:994:UNK:O	2:Q:996:UNK:N	2.35	0.60
1:D:33:CYS:SG	3:D:865:HOH:O	2.56	0.59
1:G:354:GLY:O	1:G:357:THR:HG22	2.02	0.59
1:C:193:ASN:H	1:C:318:GLN:HG2	1.66	0.59
1:K:303:ARG:NH2	1:L:547:TYR:OH	2.35	0.59
1:E:582:HIS:HE2	1:F:15:ASP:CG	2.09	0.59
1:H:234:ALA:HB1	1:H:273:ARG:NH1	2.17	0.59
1:E:584:ASN:ND2	1:F:11:ASP:OD2	2.35	0.59
2:Q:991:UNK:N	3:Q:1101:HOH:O	2.32	0.59
1:K:126:GLY:N	1:K:139:SER:OG	2.35	0.59
2:N:991:UNK:O	3:N:1101:HOH:O	2.17	0.59
1:A:174:VAL:HG23	1:A:289:GLN:HG2	1.85	0.59
1:H:187:ARG:NH1	1:H:324:ASP:OD2	2.35	0.59
1:E:187:ARG:NE	1:E:324:ASP:OD2	2.35	0.58
1:L:110:ALA:O	3:L:701:HOH:O	2.17	0.58
1:L:439:LEU:HD13	1:L:443:VAL:HG21	1.84	0.58
1:H:51:GLU:HA	1:H:54:HIS:O	2.04	0.58
1:E:415:THR:HG22	1:E:618:LEU:HB3	1.85	0.58
1:B:182:LEU:O	3:B:701:HOH:O	2.17	0.58
1:D:102:MET:SD	1:D:321:ILE:HD11	2.44	0.58
1:L:590:GLU:OE1	1:L:590:GLU:N	2.37	0.58
1:C:182:LEU:HD22	1:C:205:ALA:HB1	1.86	0.57
1:A:101:ASP:HB3	1:A:303:ARG:HG3	1.86	0.57
1:G:75:THR:HG21	1:G:93:PRO:CG	2.32	0.57
1:L:533:ILE:HD13	1:L:587:ARG:HH21	1.69	0.57
1:K:51:GLU:OE1	3:K:702:HOH:O	2.17	0.57
1:A:585:ILE:HG22	1:B:11:ASP:HB3	1.85	0.57
1:L:178:GLU:HG3	1:L:465:ARG:HA	1.85	0.57
1:E:440:LYS:HD2	1:E:441:TRP:H	1.70	0.57
1:J:584:ASN:ND2	1:K:15:ASP:OD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:520:THR:OG1	3:E:701:HOH:O	2.18	0.56
1:G:59:ASN:O	3:G:701:HOH:O	2.18	0.56
1:I:183:ARG:HB2	1:I:467:TRP:CZ2	2.41	0.56
1:K:589:ARG:O	1:K:591:PHE:N	2.38	0.56
1:F:27:ARG:HA	2:R:994:UNK:CB	2.35	0.56
1:F:584:ASN:O	1:F:588:ALA:N	2.36	0.56
1:A:189:LYS:HE2	1:A:191:GLU:HG2	1.86	0.56
1:K:584:ASN:HD22	1:L:15:ASP:CG	2.14	0.56
1:A:175:ARG:HE	1:A:464:TRP:CG	2.23	0.56
1:A:175:ARG:HH21	1:A:464:TRP:CD1	2.23	0.56
1:G:313:SER:HB3	1:G:620:ILE:HG23	1.88	0.56
1:H:28:ILE:HG22	1:H:32:MET:HE2	1.87	0.56
1:G:51:GLU:HA	1:G:54:HIS:O	2.05	0.56
1:C:442:PRO:HB3	1:C:582:HIS:CD2	2.40	0.55
1:E:4:VAL:N	1:F:71:GLU:OE1	2.38	0.55
1:A:235:SER:HB3	1:B:514:TYR:CE1	2.40	0.55
1:E:27:ARG:NH2	1:E:49:ASP:O	2.35	0.55
1:G:33:CYS:SG	3:G:854:HOH:O	2.58	0.55
1:H:383:ASP:OD1	1:H:385:THR:OG1	2.24	0.55
1:B:51:GLU:HA	1:B:54:HIS:O	2.05	0.55
1:H:37:LYS:NZ	3:H:720:HOH:O	2.39	0.55
1:A:334:THR:HG23	1:A:382:ILE:HG23	1.89	0.55
1:E:27:ARG:HH11	2:Q:995:UNK:HA	1.72	0.55
1:F:193:ASN:HA	1:F:318:GLN:NE2	2.22	0.55
1:A:42:ASP:OD2	1:B:411:ARG:NH2	2.39	0.55
1:C:408:TYR:CE1	1:C:412:ILE:HD11	2.42	0.55
1:D:13:LYS:NZ	3:D:715:HOH:O	2.39	0.55
1:B:439:LEU:HD13	1:B:443:VAL:HG21	1.89	0.54
1:A:175:ARG:NH2	3:A:706:HOH:O	2.32	0.54
1:B:344:THR:HG22	1:B:370:THR:OG1	2.08	0.54
1:D:63:LYS:HB2	1:F:55:ILE:HG13	1.89	0.54
1:H:364:THR:HG22	1:H:365:GLN:HG3	1.90	0.54
1:I:221:TRP:O	1:I:225:ILE:HG13	2.07	0.54
2:X:1005:UNK:N	3:X:1101:HOH:O	2.33	0.54
1:D:52:ARG:NH2	2:P:996:UNK:O	2.41	0.54
1:G:487:ARG:HB3	1:G:502:PHE:CE1	2.43	0.54
1:E:342:GLN:OE1	3:E:702:HOH:O	2.18	0.54
1:L:13:LYS:HG2	1:L:16:ARG:NH2	2.23	0.54
1:E:28:ILE:HG22	1:E:32:MET:HE2	1.89	0.54
1:G:524:ASP:HB2	1:G:596:THR:HG22	1.90	0.54
1:J:255:ASP:OD1	1:J:259:THR:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:TYR:CE1	1:C:235:SER:HB3	2.43	0.53
1:C:347:THR:OG1	1:C:367:ASN:HB2	2.09	0.53
1:D:27:ARG:NH2	1:D:49:ASP:O	2.41	0.53
1:I:92:ILE:HG23	1:I:395:ILE:HD13	1.89	0.53
1:B:46:THR:HA	1:C:411:ARG:HH11	1.72	0.53
1:J:52:ARG:NH2	2:V:996:UNK:O	2.41	0.53
1:J:326:GLU:OE1	3:J:701:HOH:O	2.18	0.53
1:E:303:ARG:NH1	1:F:551:ASN:OD1	2.37	0.53
1:K:51:GLU:HA	1:K:54:HIS:O	2.09	0.53
1:A:24:LEU:HB2	1:A:54:HIS:CE1	2.44	0.53
1:E:13:LYS:HG2	1:E:17:MET:HE2	1.91	0.53
1:B:312:VAL:HG11	1:B:409:ILE:HG12	1.91	0.53
1:I:573:TYR:O	1:I:576:THR:OG1	2.24	0.53
1:K:89:GLN:HG3	1:K:322:THR:HG22	1.91	0.53
1:A:432:ASP:OD1	1:A:433:GLN:N	2.42	0.53
1:H:392:GLU:OE1	3:H:701:HOH:O	2.19	0.52
1:J:357:THR:HG22	1:J:359:THR:H	1.74	0.52
1:G:58:ILE:HD11	1:H:398:ILE:HG21	1.91	0.52
1:G:221:TRP:O	1:G:225:ILE:HG13	2.09	0.52
1:H:221:TRP:O	1:H:225:ILE:HG13	2.09	0.52
1:B:364:THR:HG22	1:B:365:GLN:HG3	1.91	0.52
1:E:490:ILE:HD13	1:E:503:LYS:HE2	1.92	0.52
1:A:46:THR:HG22	1:A:48:VAL:N	2.22	0.52
1:C:24:LEU:HB2	1:C:54:HIS:CE1	2.44	0.52
1:C:102:MET:HE2	1:C:395:ILE:HG12	1.92	0.52
1:E:105:HIS:O	1:E:391:ILE:HA	2.09	0.52
1:E:238:VAL:HG11	1:E:274:LYS:HE3	1.92	0.52
1:L:48:VAL:O	1:L:52:ARG:HG3	2.10	0.52
1:F:48:VAL:O	1:F:52:ARG:HG3	2.09	0.52
1:B:620:ILE:HG22	1:B:621:SER:HB3	1.92	0.52
1:C:28:ILE:HA	1:C:31:ILE:HG22	1.90	0.52
1:D:51:GLU:HA	1:D:54:HIS:O	2.10	0.52
1:G:82:PRO:HG3	1:G:391:ILE:HG22	1.92	0.52
1:E:436:GLN:HB2	1:E:591:PHE:HB3	1.92	0.52
1:F:585:ILE:H	1:F:585:ILE:HD12	1.75	0.51
1:H:235:SER:HB3	1:I:514:TYR:CE2	2.45	0.51
1:J:275:LEU:HB2	1:K:277:GLN:HB2	1.92	0.51
1:A:301:TRP:H	1:A:301:TRP:CD1	2.26	0.51
1:G:92:ILE:HG23	1:G:395:ILE:HD13	1.92	0.51
1:A:527:ARG:NH1	1:A:529:LYS:HE2	2.18	0.51
1:D:235:SER:HB3	1:E:514:TYR:CD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:31:ILE:HG13	3:W:1101:HOH:O	2.10	0.51
1:A:175:ARG:HE	1:A:464:TRP:CD1	2.29	0.51
1:G:291:GLN:NE2	1:G:389:GLN:OE1	2.39	0.51
1:I:585:ILE:HA	1:I:588:ALA:HB3	1.91	0.51
1:C:487:ARG:HB3	1:C:502:PHE:CE1	2.46	0.51
1:H:182:LEU:HD22	1:H:205:ALA:HB1	1.92	0.51
1:H:529:LYS:NZ	3:H:726:HOH:O	2.43	0.51
1:E:58:ILE:HD11	1:F:398:ILE:HG21	1.92	0.51
1:L:545:ARG:HD2	1:L:563:LYS:HA	1.92	0.51
1:J:182:LEU:HD22	1:J:205:ALA:HB1	1.93	0.51
1:B:350:THR:HB	3:B:703:HOH:O	2.11	0.51
1:C:487:ARG:NE	1:C:504:GLN:HG2	2.26	0.50
1:E:172:ASN:ND2	1:E:380:SER:HB3	2.25	0.50
1:G:432:ASP:OD1	1:G:433:GLN:N	2.44	0.50
1:A:527:ARG:NH1	1:A:529:LYS:CG	2.74	0.50
1:D:102:MET:HG2	1:D:395:ILE:HG12	1.93	0.50
1:E:13:LYS:HE3	2:Q:1009:UNK:O	2.12	0.50
1:G:409:ILE:HG23	1:G:620:ILE:HG21	1.92	0.50
1:F:613:LYS:NZ	3:F:708:HOH:O	2.31	0.50
1:J:44:THR:O	1:K:411:ARG:NH2	2.29	0.50
1:A:24:LEU:HD21	1:B:404:ILE:HD11	1.92	0.50
1:A:407:ILE:HG12	1:C:45:PRO:HD2	1.92	0.50
1:B:487:ARG:HD3	1:B:502:PHE:CZ	2.46	0.50
1:F:183:ARG:HB2	1:F:467:TRP:CZ2	2.46	0.50
1:I:51:GLU:HA	1:I:54:HIS:O	2.12	0.50
1:A:132:LEU:HD13	1:A:137:VAL:HG22	1.93	0.50
1:D:57:LEU:HD13	1:F:572:LEU:HD12	1.93	0.50
1:G:486:ALA:HB3	1:G:505:SER:HB3	1.93	0.50
1:K:31:ILE:O	1:K:35:ARG:HG3	2.11	0.50
1:E:79:THR:HG21	1:E:88:ILE:HA	1.93	0.50
1:C:183:ARG:HB2	1:C:467:TRP:CZ2	2.47	0.50
1:K:6:LYS:HE3	1:K:8:ILE:HD11	1.94	0.50
1:K:157:VAL:HG12	1:K:158:ASN:O	2.11	0.50
1:A:487:ARG:HB3	1:A:502:PHE:CE1	2.47	0.50
1:H:16:ARG:NH2	3:H:712:HOH:O	2.32	0.50
1:L:92:ILE:HG23	1:L:395:ILE:HD13	1.94	0.50
1:G:27:ARG:O	1:G:31:ILE:HG22	2.12	0.50
1:J:587:ARG:HH21	1:K:6:LYS:HE3	1.77	0.49
2:R:991:UNK:HA	3:R:1102:HOH:O	2.12	0.49
1:J:540:ARG:NH2	3:J:715:HOH:O	2.41	0.49
2:X:1006:UNK:N	3:X:1101:HOH:O	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:THR:OG1	1:A:367:ASN:HB2	2.11	0.49
1:I:154:GLN:HA	1:I:342:GLN:O	2.11	0.49
1:G:235:SER:HB3	1:H:514:TYR:CE1	2.48	0.49
1:B:105:HIS:O	1:B:391:ILE:HA	2.13	0.49
1:B:478:VAL:HB	1:B:514:TYR:HB2	1.94	0.49
1:F:30:SER:OG	2:R:994:UNK:O	2.29	0.49
1:F:46:THR:OG1	1:F:49:ASP:N	2.41	0.49
1:F:439:LEU:HD13	1:F:443:VAL:HG21	1.95	0.49
1:D:140:ALA:HB2	1:D:151:LEU:HD12	1.95	0.49
1:D:530:ALA:O	1:D:533:ILE:HG13	2.13	0.49
1:I:553:GLY:HA2	1:I:574:PRO:O	2.13	0.49
1:J:514:TYR:CE2	1:L:235:SER:HB3	2.48	0.48
1:K:28:ILE:HG22	1:K:32:MET:HE2	1.94	0.48
1:K:189:LYS:HG2	1:K:191:GLU:HG3	1.95	0.48
1:A:471:THR:HB	1:A:520:THR:O	2.13	0.48
1:B:383:ASP:OD1	1:B:385:THR:OG1	2.30	0.48
1:C:418:ARG:NH2	1:C:577:TYR:O	2.45	0.48
1:J:439:LEU:HD13	1:J:443:VAL:HG21	1.94	0.48
1:C:530:ALA:O	1:C:533:ILE:HG12	2.14	0.48
1:F:209:ASN:OD1	1:F:221:TRP:NE1	2.40	0.48
1:G:398:ILE:HG21	1:I:58:ILE:HD11	1.94	0.48
1:E:45:PRO:HG2	1:F:407:ILE:HD13	1.96	0.48
1:C:318:GLN:HG2	1:C:318:GLN:O	2.13	0.48
1:D:44:THR:C	1:E:411:ARG:HH21	2.18	0.48
1:F:105:HIS:O	1:F:391:ILE:HA	2.14	0.48
1:K:188:VAL:HG11	1:K:298:LEU:HD22	1.94	0.48
1:I:152:TYR:HD1	1:I:345:VAL:HG22	1.79	0.48
1:I:421:ARG:HD3	1:I:441:TRP:CZ3	2.49	0.48
1:A:221:TRP:O	1:A:225:ILE:HG13	2.14	0.48
1:A:486:ALA:HB3	1:A:505:SER:HB3	1.95	0.48
1:D:432:ASP:OD1	1:D:433:GLN:N	2.46	0.48
1:I:435:LEU:HD13	1:I:592:TYR:HE1	1.79	0.48
1:D:405:HIS:O	1:D:409:ILE:HG12	2.14	0.48
1:L:533:ILE:HD13	1:L:587:ARG:NH2	2.28	0.48
1:A:44:THR:HG21	1:B:410:LYS:HD2	1.96	0.48
1:A:527:ARG:NH2	1:A:529:LYS:HE2	2.28	0.48
1:E:228:GLU:OE2	1:E:284:THR:HG23	2.13	0.48
1:G:620:ILE:HA	1:G:621:SER:HA	1.64	0.48
1:I:193:ASN:ND2	1:I:318:GLN:OE1	2.46	0.48
1:D:270:ILE:HG12	1:F:476:GLU:HG2	1.95	0.48
1:C:545:ARG:NH1	1:C:546:ASP:OD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:PRO:HG3	1:F:585:ILE:HD11	1.96	0.47
1:I:28:ILE:HG22	1:I:32:MET:HE2	1.97	0.47
1:J:82:PRO:HG3	1:J:391:ILE:HG22	1.96	0.47
1:L:105:HIS:O	1:L:391:ILE:HA	2.14	0.47
1:C:414:PHE:HB3	1:C:619:LEU:HD23	1.95	0.47
1:L:141:THR:HG23	1:L:152:TYR:HE2	1.80	0.47
1:L:183:ARG:HB2	1:L:467:TRP:CZ2	2.49	0.47
1:A:407:ILE:HD13	1:C:50:ILE:HD11	1.97	0.47
1:G:27:ARG:HA	2:S:994:UNK:CB	2.44	0.47
1:A:527:ARG:NH1	1:A:529:LYS:HG3	2.29	0.47
1:B:477:PRO:HB3	1:B:513:GLN:HE21	1.80	0.47
1:C:412:ILE:HG21	1:C:412:ILE:HD13	1.72	0.47
1:E:192:VAL:HG13	1:E:314:ILE:HG23	1.95	0.47
1:A:175:ARG:NH1	1:A:335:ALA:HB2	2.25	0.47
1:B:182:LEU:HD22	1:B:205:ALA:HB1	1.95	0.47
1:C:456:ILE:HA	1:C:463:GLN:HG3	1.97	0.47
1:F:569:ASN:ND2	1:F:571:CYS:O	2.43	0.47
1:K:172:ASN:ND2	1:K:380:SER:HB3	2.30	0.47
1:A:362:LEU:HD23	1:A:362:LEU:O	2.14	0.47
1:G:487:ARG:HB2	1:I:366:TYR:CD2	2.49	0.47
1:I:201:THR:OG1	1:I:422:GLU:OE1	2.27	0.47
1:A:527:ARG:HH12	1:A:529:LYS:CG	2.28	0.47
1:C:51:GLU:HA	1:C:54:HIS:O	2.15	0.47
1:D:152:TYR:HD1	1:D:345:VAL:HG22	1.80	0.47
1:H:360:GLY:O	1:I:496:PRO:HD2	2.14	0.47
1:K:44:THR:HG21	1:L:410:LYS:HD3	1.95	0.47
1:K:415:THR:OG1	1:K:618:LEU:HB3	2.14	0.47
1:L:24:LEU:O	1:L:28:ILE:HG12	2.15	0.47
1:L:27:ARG:NH2	1:L:49:ASP:O	2.45	0.47
1:D:60:SER:OG	1:E:412:ILE:HD11	2.14	0.47
1:G:572:LEU:HD12	1:H:57:LEU:HD13	1.96	0.47
1:H:24:LEU:HD21	1:I:404:ILE:HD11	1.97	0.47
1:J:414:PHE:HB3	1:J:619:LEU:HD23	1.97	0.47
1:F:531:HIS:CD2	1:F:587:ARG:HA	2.50	0.47
1:I:351:THR:OG1	1:I:362:LEU:HD22	2.15	0.47
1:J:235:SER:HB3	1:K:514:TYR:CE2	2.50	0.47
2:W:993:UNK:O	2:W:995:UNK:N	2.48	0.47
1:A:412:ILE:CG2	1:A:620:ILE:HG13	2.44	0.47
1:I:301:TRP:H	1:I:301:TRP:CD1	2.32	0.47
1:A:62:TYR:CE1	1:B:416:LEU:HD13	2.50	0.46
1:B:94:GLN:HE22	1:D:315:PRO:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:PRO:HG3	1:C:391:ILE:HG22	1.97	0.46
1:I:50:ILE:HG21	1:I:56:LEU:HD21	1.97	0.46
1:F:285:PRO:HB3	1:F:335:ALA:HB3	1.98	0.46
1:G:373:THR:O	1:G:375:THR:HG23	2.15	0.46
1:I:13:LYS:O	1:I:17:MET:HG3	2.16	0.46
1:J:152:TYR:HD1	1:J:345:VAL:HG22	1.79	0.46
1:L:102:MET:O	1:L:303:ARG:NH2	2.48	0.46
1:B:347:THR:OG1	1:B:367:ASN:HB2	2.16	0.46
1:K:57:LEU:HD12	1:L:68:MET:HE2	1.97	0.46
1:K:187:ARG:NH2	1:K:324:ASP:OD2	2.48	0.46
1:C:352:GLY:HA3	1:C:361:VAL:HG23	1.96	0.46
1:F:111:THR:HG21	1:F:386:GLN:HB2	1.96	0.46
1:J:105:HIS:O	1:J:391:ILE:HA	2.16	0.46
1:J:189:LYS:HD2	1:J:191:GLU:HG3	1.95	0.46
1:K:189:LYS:NZ	1:K:322:THR:OG1	2.46	0.46
1:L:442:PRO:HD3	1:L:585:ILE:HG12	1.96	0.46
1:D:60:SER:HB2	1:E:415:THR:OG1	2.16	0.46
1:D:238:VAL:HG11	1:D:274:LYS:HE2	1.98	0.46
1:D:529:LYS:HG2	1:D:592:TYR:HB2	1.98	0.46
1:F:346:GLU:OE1	1:F:366:TYR:OH	2.30	0.46
1:J:587:ARG:HH21	1:K:6:LYS:CE	2.29	0.46
1:C:537:ALA:HB3	1:C:539:TYR:CZ	2.51	0.46
1:G:149:TYR:HD2	1:G:348:LEU:HD12	1.81	0.46
1:C:221:TRP:O	1:C:225:ILE:HG12	2.14	0.46
1:C:411:ARG:HA	1:C:411:ARG:HD3	1.71	0.46
1:D:398:ILE:HG21	1:F:58:ILE:HD11	1.97	0.46
1:E:411:ARG:HD3	1:E:411:ARG:HA	1.75	0.46
1:L:203:LEU:HD13	1:L:609:ILE:HG12	1.96	0.46
1:C:334:THR:HG21	1:C:381:SER:HA	1.98	0.46
1:E:157:VAL:HG12	1:E:158:ASN:O	2.15	0.46
1:I:544:TYR:HB2	1:I:566:LEU:HD23	1.98	0.46
1:D:604:ASN:ND2	3:D:707:HOH:O	2.33	0.46
1:J:197:LEU:HD11	1:J:618:LEU:HD11	1.97	0.46
1:K:95:PHE:HB3	1:K:397:ASN:OD1	2.16	0.46
1:K:180:PRO:HD2	1:K:225:ILE:O	2.15	0.46
1:K:295:PHE:O	1:K:297:PRO:HD3	2.16	0.46
1:G:135:THR:HB	1:G:163:THR:HG21	1.97	0.46
1:G:416:LEU:HD21	1:G:615:ILE:HG23	1.97	0.46
1:H:442:PRO:HA	1:H:583:VAL:O	2.16	0.46
1:J:51:GLU:HA	1:J:54:HIS:O	2.16	0.46
1:B:531:HIS:O	1:B:531:HIS:ND1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:GLN:HA	1:F:342:GLN:O	2.15	0.45
1:J:398:ILE:HG21	1:L:58:ILE:HD11	1.97	0.45
1:K:183:ARG:HB2	1:K:467:TRP:CZ2	2.51	0.45
1:I:530:ALA:O	1:I:533:ILE:HG13	2.15	0.45
1:B:221:TRP:O	1:B:225:ILE:HG12	2.16	0.45
1:B:438:GLN:HG2	1:B:439:LEU:HD23	1.99	0.45
1:K:76:ARG:HH12	1:K:390:ASN:ND2	2.13	0.45
1:K:124:PHE:CE1	1:K:130:GLN:HB3	2.52	0.45
1:G:31:ILE:HG23	1:G:45:PRO:HG3	1.97	0.45
1:H:503:LYS:HG3	1:I:488:VAL:HG13	1.97	0.45
1:B:31:ILE:O	1:B:35:ARG:HG3	2.15	0.45
1:H:587:ARG:NH2	1:I:6:LYS:O	2.38	0.45
1:J:255:ASP:OD1	1:J:258:GLY:N	2.49	0.45
1:J:540:ARG:NH1	3:J:724:HOH:O	2.49	0.45
1:A:215:ASP:HA	1:A:218:LEU:HB2	1.99	0.45
1:D:321:ILE:HD12	1:D:393:LEU:HD21	1.98	0.45
1:F:491:ASP:HB3	1:F:494:VAL:HG22	1.99	0.45
1:H:347:THR:OG1	1:H:367:ASN:HB2	2.17	0.45
1:B:177:CYS:O	1:B:180:PRO:HD3	2.16	0.45
1:B:432:ASP:OD1	1:B:433:GLN:N	2.46	0.45
1:F:585:ILE:HA	1:F:588:ALA:HB3	1.99	0.45
1:I:190:PHE:CE2	1:I:197:LEU:HD23	2.52	0.45
1:K:221:TRP:O	1:K:225:ILE:HG12	2.17	0.45
1:K:418:ARG:HE	1:K:444:GLU:CD	2.25	0.45
1:C:156:TYR:HB3	1:C:339:LEU:HD11	1.98	0.45
1:C:203:LEU:HB3	1:C:611:ILE:HD11	1.98	0.45
1:J:189:LYS:HD3	1:J:196:PRO:HB3	1.99	0.45
1:D:112:SER:HB3	1:D:288:THR:HG22	1.99	0.45
1:F:121:LEU:HD13	1:F:137:VAL:HG23	1.99	0.45
1:G:95:PHE:HB3	1:G:397:ASN:OD1	2.17	0.45
1:K:46:THR:HG23	1:K:49:ASP:H	1.82	0.45
1:L:121:LEU:HD13	1:L:137:VAL:HG23	1.98	0.45
1:L:135:THR:HB	1:L:163:THR:HG21	1.99	0.45
1:H:477:PRO:HB3	1:H:513:GLN:HE21	1.81	0.44
1:D:96:GLY:HA2	1:D:399:PHE:CE1	2.52	0.44
1:E:63:LYS:HG3	1:E:64:PRO:HD2	1.98	0.44
1:G:182:LEU:HD21	1:G:221:TRP:HZ2	1.81	0.44
1:L:75:THR:HG21	1:L:93:PRO:CG	2.47	0.44
1:D:189:LYS:HD2	1:D:191:GLU:HG2	1.99	0.44
1:D:480:ASP:OD1	1:E:274:LYS:NZ	2.42	0.44
1:J:187:ARG:NH1	1:J:324:ASP:OD2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:442:PRO:HB3	1:J:582:HIS:CD2	2.52	0.44
1:J:448:LEU:HD11	1:J:608:LEU:HD11	1.99	0.44
1:E:295:PHE:O	1:E:297:PRO:HD3	2.16	0.44
1:A:487:ARG:HB2	1:C:366:TYR:CD2	2.52	0.44
1:D:255:ASP:OD1	1:D:258:GLY:N	2.51	0.44
1:G:134:SER:HB2	1:G:165:THR:HG23	1.99	0.44
1:G:440:LYS:O	1:G:585:ILE:HD11	2.17	0.44
1:I:29:LYS:HG3	1:I:30:SER:N	2.32	0.44
1:K:101:ASP:HB2	1:K:303:ARG:NH2	2.32	0.44
1:B:51:GLU:O	1:C:63:LYS:NZ	2.48	0.44
1:D:189:LYS:HD2	1:D:191:GLU:CG	2.47	0.44
1:H:94:GLN:OE1	1:J:315:PRO:HA	2.18	0.44
1:J:27:ARG:HD2	2:V:994:UNK:O	2.18	0.44
1:L:412:ILE:CG2	1:L:620:ILE:HG13	2.47	0.44
1:H:95:PHE:HB3	1:H:397:ASN:OD1	2.18	0.44
1:A:279:VAL:HG13	1:C:275:LEU:HD21	2.00	0.44
1:B:47:LEU:HD11	1:C:412:ILE:HG13	1.99	0.44
1:E:613:LYS:NZ	3:E:732:HOH:O	2.51	0.44
1:F:406:ASP:OD2	1:F:410:LYS:NZ	2.50	0.44
1:G:124:PHE:CZ	1:G:130:GLN:HB3	2.53	0.44
1:I:124:PHE:CE1	1:I:130:GLN:HB3	2.53	0.44
1:D:304:ASP:OD1	1:D:306:ARG:HG2	2.17	0.44
1:E:24:LEU:HD21	1:F:404:ILE:HD11	2.00	0.44
1:L:51:GLU:HA	1:L:54:HIS:O	2.18	0.44
1:B:192:VAL:HG21	1:B:314:ILE:HD13	2.01	0.43
1:B:371:THR:HB	1:B:510:MET:HE3	1.99	0.43
1:I:545:ARG:HD2	1:I:546:ASP:OD1	2.18	0.43
1:B:312:VAL:HG23	1:D:317:GLY:CA	2.47	0.43
1:E:174:VAL:HG23	1:E:289:GLN:HG2	1.99	0.43
1:F:527:ARG:HD3	1:F:594:GLU:OE2	2.17	0.43
1:H:315:PRO:HB3	1:J:318:GLN:OE1	2.17	0.43
1:I:436:GLN:HB2	1:I:591:PHE:HB3	2.00	0.43
1:I:613:LYS:HD2	1:I:613:LYS:HA	1.73	0.43
1:L:326:GLU:OE1	3:L:703:HOH:O	2.21	0.43
1:A:589:ARG:O	1:A:589:ARG:HG2	2.18	0.43
1:H:289:GLN:OE1	3:H:702:HOH:O	2.20	0.43
1:I:529:LYS:HE2	1:I:532:GLY:HA2	2.00	0.43
1:L:75:THR:HG21	1:L:93:PRO:HG2	2.01	0.43
1:B:235:SER:HB3	1:C:514:TYR:CE2	2.54	0.43
1:E:183:ARG:HB2	1:E:467:TRP:CZ2	2.53	0.43
1:F:422:GLU:HG3	1:F:611:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:285:PRO:HB3	1:L:335:ALA:HB3	1.99	0.43
1:L:485:TYR:O	3:L:702:HOH:O	2.21	0.43
2:X:1002:UNK:C	3:X:1101:HOH:O	2.66	0.43
1:B:459:GLY:N	3:B:716:HOH:O	2.31	0.43
1:C:154:GLN:HA	1:C:342:GLN:O	2.19	0.43
1:D:531:HIS:HB2	1:D:587:ARG:HA	2.00	0.43
1:B:466:ASP:OD2	3:B:702:HOH:O	2.21	0.43
1:I:477:PRO:HB3	1:I:513:GLN:NE2	2.34	0.43
1:J:404:ILE:HD11	1:L:24:LEU:HD21	2.00	0.43
1:L:101:ASP:HB2	1:L:303:ARG:NH1	2.33	0.43
1:L:415:THR:HG23	1:L:618:LEU:HB2	2.00	0.43
1:A:51:GLU:HA	1:A:54:HIS:O	2.19	0.43
1:B:30:SER:O	1:B:34:LEU:HD13	2.18	0.43
1:G:309:ILE:HG21	1:G:314:ILE:HD12	2.00	0.43
1:H:212:HIS:NE2	1:H:447:TYR:OH	2.26	0.43
1:K:531:HIS:HA	1:K:590:GLU:CD	2.44	0.43
1:L:412:ILE:HG23	1:L:620:ILE:HG13	2.00	0.43
1:E:17:MET:HE3	1:E:17:MET:HB2	1.94	0.43
1:E:275:LEU:HB2	1:F:277:GLN:HB2	2.01	0.43
2:R:993:UNK:O	2:R:995:UNK:N	2.52	0.43
1:G:154:GLN:HA	1:G:342:GLN:O	2.18	0.43
1:K:96:GLY:HA2	1:K:399:PHE:CE2	2.54	0.43
1:K:292:LEU:HD21	1:K:294:MET:HE3	2.00	0.43
1:L:347:THR:OG1	1:L:367:ASN:HB2	2.18	0.43
1:C:571:CYS:HB3	1:C:581:GLY:O	2.19	0.43
1:D:154:GLN:HA	1:D:342:GLN:O	2.19	0.43
1:E:499:SER:OG	1:E:501:THR:HG22	2.19	0.43
1:E:585:ILE:HD12	1:E:589:ARG:HH21	1.83	0.43
1:H:476:GLU:HG2	1:I:270:ILE:HG12	2.00	0.43
1:J:529:LYS:NZ	1:J:594:GLU:OE2	2.43	0.43
1:K:220:GLY:O	1:K:224:LEU:HG	2.19	0.43
1:B:57:LEU:HD12	1:C:68:MET:HG2	2.01	0.43
1:C:418:ARG:NH1	1:C:444:GLU:OE1	2.52	0.43
1:D:95:PHE:HB3	1:D:397:ASN:OD1	2.18	0.43
1:G:301:TRP:H	1:G:301:TRP:CD1	2.36	0.43
1:H:46:THR:HG23	1:H:49:ASP:H	1.83	0.43
1:K:24:LEU:HD21	1:L:404:ILE:HD11	2.00	0.43
1:K:108:LEU:HD12	1:K:292:LEU:HD23	2.01	0.43
3:L:834:HOH:O	2:X:991:UNK:HA	2.19	0.43
1:A:530:ALA:CB	1:A:587:ARG:HB3	2.49	0.42
1:E:585:ILE:HG13	1:E:586:SER:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:223:ARG:NH1	3:K:709:HOH:O	2.52	0.42
1:J:272:ALA:HB1	1:K:278:VAL:HG13	2.01	0.42
1:C:512:ASN:OD1	1:C:513:GLN:N	2.47	0.42
1:D:442:PRO:HB3	1:D:582:HIS:CD2	2.54	0.42
1:K:46:THR:HG22	1:K:49:ASP:CG	2.43	0.42
1:C:13:LYS:O	1:C:17:MET:HG3	2.19	0.42
1:D:487:ARG:HB3	1:D:502:PHE:CE1	2.55	0.42
1:G:23:LEU:O	1:G:27:ARG:HG3	2.20	0.42
1:J:261:VAL:HG21	1:L:125:ILE:HD12	2.01	0.42
1:J:407:ILE:CD1	1:L:45:PRO:HG2	2.49	0.42
1:K:219:THR:O	1:K:223:ARG:HG3	2.19	0.42
1:K:616:ASN:OD1	1:K:617:PHE:N	2.46	0.42
1:L:210:LYS:NZ	1:L:562:ASP:OD2	2.52	0.42
1:L:487:ARG:HD2	1:L:504:GLN:HA	2.00	0.42
1:E:57:LEU:HD12	1:F:68:MET:HE2	2.01	0.42
1:G:450:LEU:HB3	1:G:522:THR:OG1	2.19	0.42
1:J:180:PRO:HD2	1:J:225:ILE:O	2.20	0.42
1:A:404:ILE:HD11	1:C:24:LEU:HD21	2.00	0.42
1:A:416:LEU:HD11	1:A:579:PRO:HG3	2.01	0.42
1:A:474:THR:CG2	1:A:518:VAL:HB	2.49	0.42
1:C:554:SER:OG	1:C:555:PHE:N	2.53	0.42
1:G:526:VAL:HB	1:G:544:TYR:CE2	2.54	0.42
1:I:405:HIS:ND1	1:I:409:ILE:HD11	2.35	0.42
1:J:587:ARG:NH2	1:K:6:LYS:O	2.51	0.42
1:H:201:THR:OG1	1:H:422:GLU:OE1	2.31	0.42
1:H:289:GLN:HG3	3:H:724:HOH:O	2.20	0.42
1:J:55:ILE:HD11	1:K:63:LYS:HB2	2.00	0.42
1:L:487:ARG:NE	1:L:504:GLN:HG2	2.35	0.42
1:A:193:ASN:ND2	1:A:318:GLN:OE1	2.53	0.42
1:B:238:VAL:HG11	1:B:274:LYS:HD3	2.02	0.42
1:G:94:GLN:OE1	1:G:311:SER:OG	2.33	0.42
1:I:48:VAL:O	1:I:52:ARG:HG3	2.19	0.42
1:A:105:HIS:O	1:A:391:ILE:HA	2.20	0.42
1:I:537:ALA:HB3	1:I:539:TYR:CZ	2.54	0.42
1:K:55:ILE:HD12	1:K:55:ILE:HA	1.97	0.42
1:A:307:LEU:HD11	1:A:577:TYR:CD1	2.55	0.42
1:D:585:ILE:HD12	1:D:589:ARG:HH21	1.84	0.42
1:F:85:ASN:CB	1:F:327:GLN:HG2	2.48	0.42
1:H:527:ARG:NH1	1:H:534:GLU:OE2	2.51	0.42
1:A:279:VAL:HG23	1:C:273:ARG:HG3	2.01	0.42
1:D:277:GLN:HB2	1:F:275:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:315:PRO:HB3	1:J:318:GLN:CD	2.45	0.42
1:H:557:LEU:HD12	1:H:557:LEU:HA	1.90	0.42
1:C:476:GLU:HB3	1:C:516:VAL:HB	2.01	0.41
1:C:585:ILE:HG13	1:C:586:SER:N	2.33	0.41
1:D:235:SER:HB3	1:E:514:TYR:CE2	2.55	0.41
1:H:46:THR:HG22	1:H:49:ASP:CG	2.44	0.41
1:I:574:PRO:HA	1:I:575:GLY:HA2	1.70	0.41
1:K:68:MET:HE2	1:K:398:ILE:HG23	2.01	0.41
1:D:273:ARG:NE	1:E:284:THR:HG22	2.19	0.41
1:G:140:ALA:HB2	1:G:151:LEU:HD12	2.03	0.41
1:H:183:ARG:HB2	1:H:467:TRP:CZ2	2.55	0.41
1:I:24:LEU:HB2	1:I:54:HIS:CE1	2.55	0.41
1:C:31:ILE:CG2	1:C:45:PRO:HG3	2.51	0.41
1:D:82:PRO:HG3	1:D:391:ILE:HG22	2.02	0.41
1:G:407:ILE:HG12	1:I:45:PRO:HD2	2.02	0.41
1:H:6:LYS:HA	1:H:6:LYS:HD3	1.90	0.41
1:G:436:GLN:HB2	1:G:591:PHE:HB3	2.03	0.41
1:I:68:MET:HE3	1:I:68:MET:HB3	1.89	0.41
1:I:347:THR:OG1	1:I:367:ASN:HB2	2.21	0.41
1:A:527:ARG:CZ	1:A:529:LYS:CE	2.93	0.41
1:D:545:ARG:HD2	1:D:546:ASP:OD1	2.21	0.41
1:F:31:ILE:HD13	1:F:49:ASP:HB3	2.01	0.41
1:G:411:ARG:NH2	1:I:44:THR:O	2.49	0.41
1:I:200:TYR:HB2	1:I:204:ALA:HB3	2.02	0.41
1:K:174:VAL:HG23	1:K:289:GLN:HG2	2.02	0.41
1:B:133:THR:HG22	1:B:134:SER:H	1.86	0.41
1:E:216:PHE:HB2	1:F:558:VAL:HG22	2.02	0.41
1:G:346:GLU:OE1	1:G:366:TYR:OH	2.26	0.41
1:H:585:ILE:O	1:H:589:ARG:HG3	2.21	0.41
1:J:124:PHE:CE1	1:J:130:GLN:HB3	2.56	0.41
1:J:599:PHE:CE2	1:J:604:ASN:HB3	2.55	0.41
1:L:24:LEU:HD13	1:L:54:HIS:CG	2.56	0.41
1:L:154:GLN:HA	1:L:342:GLN:O	2.20	0.41
1:A:46:THR:HA	1:B:411:ARG:HD2	2.02	0.41
1:A:309:ILE:HG21	1:A:314:ILE:HD12	2.02	0.41
1:B:133:THR:HG22	1:B:134:SER:N	2.36	0.41
1:C:417:ILE:HG21	1:C:618:LEU:HD13	2.02	0.41
1:D:244:THR:HG21	1:D:251:VAL:HG21	2.03	0.41
1:D:449:GLY:HA3	1:D:470:LEU:HD13	2.02	0.41
1:E:51:GLU:HA	1:E:54:HIS:O	2.21	0.41
1:I:239:ASN:O	1:I:271:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:27:ARG:HH11	2:V:995:UNK:HA	1.84	0.41
1:K:361:VAL:O	1:K:362:LEU:HB3	2.20	0.41
1:C:105:HIS:O	1:C:391:ILE:HA	2.21	0.41
1:C:421:ARG:HD3	1:C:441:TRP:HZ3	1.86	0.41
1:G:466:ASP:OD2	3:G:702:HOH:O	2.21	0.41
1:H:416:LEU:HB2	1:H:577:TYR:CE1	2.56	0.41
1:L:434:VAL:HG11	1:L:608:LEU:HD23	2.03	0.41
1:B:239:ASN:O	1:B:271:THR:HA	2.21	0.41
1:C:186:LYS:HD2	1:C:326:GLU:HA	2.02	0.41
1:E:255:ASP:OD2	1:E:259:THR:HB	2.20	0.41
1:E:571:CYS:HB3	1:E:581:GLY:O	2.21	0.41
1:K:347:THR:OG1	1:K:367:ASN:HB2	2.21	0.41
1:L:531:HIS:NE2	1:L:586:SER:O	2.53	0.41
1:A:172:ASN:ND2	1:A:380:SER:HB3	2.35	0.41
1:B:174:VAL:HG23	1:B:289:GLN:HB2	2.01	0.41
1:B:615:ILE:HG21	1:C:18:ILE:HD11	2.03	0.41
1:C:472:SER:HB3	1:C:520:THR:HB	2.02	0.41
1:D:238:VAL:HG22	1:D:273:ARG:HA	2.02	0.41
1:E:31:ILE:O	1:E:35:ARG:HG3	2.21	0.41
1:E:450:LEU:HD13	1:E:608:LEU:HD23	2.01	0.41
1:I:102:MET:HE2	1:I:302:PHE:CZ	2.56	0.41
1:I:435:LEU:HD13	1:I:592:TYR:CE1	2.56	0.41
1:J:186:LYS:NZ	3:J:701:HOH:O	2.30	0.41
1:K:512:ASN:OD1	1:K:513:GLN:N	2.48	0.41
1:L:221:TRP:O	1:L:225:ILE:HG12	2.21	0.41
1:C:442:PRO:HD3	1:C:585:ILE:HG22	2.03	0.40
1:D:47:LEU:HD23	1:D:47:LEU:HA	1.79	0.40
1:E:426:ARG:HD3	1:E:427:GLU:H	1.86	0.40
1:I:23:LEU:O	1:I:27:ARG:HG3	2.20	0.40
1:I:477:PRO:HB3	1:I:513:GLN:HE21	1.86	0.40
1:J:24:LEU:HB2	1:J:54:HIS:CE1	2.56	0.40
2:X:1008:UNK:HA	3:X:1102:HOH:O	2.21	0.40
1:A:189:LYS:CE	1:A:196:PRO:HG3	2.49	0.40
1:B:32:MET:HE2	1:B:44:THR:HG22	2.03	0.40
1:F:463:GLN:HE21	1:F:463:GLN:HB3	1.60	0.40
1:H:124:PHE:O	1:I:255:ASP:HB2	2.21	0.40
1:H:275:LEU:HD12	1:I:230:PRO:HB3	2.03	0.40
1:I:515:ILE:HD13	1:I:515:ILE:HA	1.97	0.40
1:J:304:ASP:OD1	1:J:306:ARG:HG2	2.20	0.40
1:B:46:THR:HA	1:C:411:ARG:NH1	2.36	0.40
1:B:95:PHE:HB3	1:B:397:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ARG:HB2	1:B:467:TRP:CZ2	2.56	0.40
1:B:487:ARG:HG2	1:B:503:LYS:O	2.22	0.40
1:C:423:GLN:OE1	1:C:437:SER:N	2.54	0.40
1:C:440:LYS:HZ2	1:C:441:TRP:NE1	2.20	0.40
1:F:416:LEU:HD12	1:F:617:PHE:CE1	2.56	0.40
1:H:235:SER:O	1:H:273:ARG:HD2	2.21	0.40
1:J:476:GLU:HG2	1:K:270:ILE:HG12	2.04	0.40
1:L:154:GLN:HG2	1:L:343:THR:HA	2.03	0.40
1:L:238:VAL:HG11	1:L:274:LYS:HD2	2.02	0.40
1:B:613:LYS:HA	1:B:613:LYS:HD2	1.79	0.40
1:E:221:TRP:O	1:E:225:ILE:HG12	2.21	0.40
1:E:445:PHE:CE1	1:E:613:LYS:HG3	2.57	0.40
1:H:601:ASP:OD1	1:H:603:SER:N	2.55	0.40
1:I:294:MET:HB2	1:I:294:MET:HE3	1.88	0.40
1:K:225:ILE:O	1:K:294:MET:HE2	2.21	0.40
1:B:30:SER:OG	2:N:992:UNK:O	2.26	0.40
1:E:383:ASP:OD1	1:E:385:THR:OG1	2.26	0.40
1:F:530:ALA:HB1	1:F:587:ARG:O	2.22	0.40
1:H:24:LEU:O	1:H:28:ILE:HG13	2.22	0.40
1:J:206:ILE:O	1:J:210:LYS:HG3	2.21	0.40
1:K:149:TYR:CZ	1:K:358:ALA:HB2	2.56	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	607/645 (94%)	593 (98%)	14 (2%)	0	100	100
1	B	614/645 (95%)	597 (97%)	17 (3%)	0	100	100
1	C	614/645 (95%)	598 (97%)	16 (3%)	0	100	100
1	D	607/645 (94%)	591 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	614/645 (95%)	597 (97%)	17 (3%)	0	100	100
1	F	608/645 (94%)	583 (96%)	25 (4%)	0	100	100
1	G	609/645 (94%)	592 (97%)	17 (3%)	0	100	100
1	H	613/645 (95%)	593 (97%)	20 (3%)	0	100	100
1	I	614/645 (95%)	596 (97%)	18 (3%)	0	100	100
1	J	608/645 (94%)	592 (97%)	16 (3%)	0	100	100
1	K	612/645 (95%)	590 (96%)	21 (3%)	1 (0%)	43	53
1	L	608/645 (94%)	588 (97%)	20 (3%)	0	100	100
All	All	7328/7740 (95%)	7110 (97%)	217 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	590	GLU

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	524/554 (95%)	523 (100%)	1 (0%)	87	92
1	B	530/554 (96%)	530 (100%)	0	100	100
1	C	530/554 (96%)	530 (100%)	0	100	100
1	D	524/554 (95%)	524 (100%)	0	100	100
1	E	530/554 (96%)	529 (100%)	1 (0%)	87	92
1	F	525/554 (95%)	525 (100%)	0	100	100
1	G	526/554 (95%)	525 (100%)	1 (0%)	87	92
1	H	529/554 (96%)	529 (100%)	0	100	100
1	I	530/554 (96%)	530 (100%)	0	100	100
1	J	525/554 (95%)	525 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	528/554 (95%)	528 (100%)	0	100	100
1	L	525/554 (95%)	525 (100%)	0	100	100
All	All	6326/6648 (95%)	6323 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	MET
1	E	416	LEU
1	G	68	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	89	GLN
1	A	154	GLN
1	A	193	ASN
1	B	38	GLN
1	B	59	ASN
1	B	73	GLN
1	B	429	ASN
1	B	513	GLN
1	C	78	ASN
1	C	85	ASN
1	C	89	GLN
1	C	367	ASN
1	C	438	GLN
1	C	454	ASN
1	D	21	ASN
1	D	107	GLN
1	D	160	GLN
1	D	193	ASN
1	D	291	GLN
1	D	293	ASN
1	D	342	GLN
1	D	433	GLN
1	D	454	ASN
1	D	511	GLN
1	D	556	ASN

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Mol	Chain	Res	Type
1	E	107	GLN
1	E	405	HIS
1	E	511	GLN
1	E	604	ASN
1	F	21	ASN
1	F	61	HIS
1	F	73	GLN
1	F	81	ASN
1	F	193	ASN
1	F	277	GLN
1	F	511	GLN
1	F	556	ASN
1	G	107	GLN
1	G	277	GLN
1	G	483	GLN
1	G	511	GLN
1	H	38	GLN
1	H	73	GLN
1	H	429	ASN
1	H	511	GLN
1	H	513	GLN
1	I	78	ASN
1	I	89	GLN
1	I	107	GLN
1	I	154	GLN
1	I	291	GLN
1	I	293	ASN
1	I	511	GLN
1	I	513	GLN
1	J	164	GLN
1	J	277	GLN
1	J	429	ASN
1	J	454	ASN
1	J	511	GLN
1	J	513	GLN
1	K	61	HIS
1	K	78	ASN
1	K	89	GLN
1	K	130	GLN
1	K	193	ASN
1	K	390	ASN
1	K	511	GLN

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Mol	Chain	Res	Type
1	L	25	ASN
1	L	73	GLN
1	L	195	ASN
1	L	277	GLN
1	L	318	GLN
1	L	367	ASN
1	L	405	HIS
1	L	511	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	609/645 (94%)	-0.12	6 (0%) 79 81	24, 39, 59, 72	0
1	B	616/645 (95%)	-0.10	7 (1%) 78 79	24, 39, 62, 93	0
1	C	616/645 (95%)	-0.04	24 (3%) 43 40	26, 40, 67, 112	0
1	D	609/645 (94%)	-0.09	4 (0%) 84 85	27, 40, 61, 84	0
1	E	616/645 (95%)	0.10	23 (3%) 45 43	29, 42, 72, 120	0
1	F	610/645 (94%)	-0.01	14 (2%) 61 62	24, 39, 66, 127	0
1	G	611/645 (94%)	-0.04	4 (0%) 84 85	26, 41, 63, 93	0
1	H	615/645 (95%)	-0.10	11 (1%) 67 68	23, 40, 65, 98	0
1	I	616/645 (95%)	0.15	21 (3%) 48 46	29, 46, 70, 123	0
1	J	610/645 (94%)	-0.14	3 (0%) 87 89	25, 39, 65, 85	0
1	K	614/645 (95%)	0.06	16 (2%) 57 57	29, 43, 72, 106	0
1	L	610/645 (94%)	-0.03	12 (1%) 65 66	26, 41, 65, 116	0
2	M	0/21	-	-	-	-
2	N	0/21	-	-	-	-
2	O	0/21	-	-	-	-
2	P	0/21	-	-	-	-
2	Q	0/21	-	-	-	-
2	R	0/21	-	-	-	-
2	S	0/21	-	-	-	-
2	T	0/21	-	-	-	-
2	U	0/21	-	-	-	-
2	V	0/21	-	-	-	-
2	W	0/21	-	-	-	-
2	X	0/21	-	-	-	-
All	All	7352/7992 (91%)	-0.03	145 (1%) 65 66	23, 41, 65, 127	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	588	ALA	8.2
1	E	585	ILE	6.4
1	C	588	ALA	6.0
1	K	588	ALA	4.9
1	E	588	ALA	4.8
1	I	5	PHE	4.8
1	I	587	ARG	4.8
1	I	585	ILE	4.7
1	K	80	GLY	4.7
1	C	584	ASN	4.7
1	I	620	ILE	4.5
1	I	590	GLU	4.5
1	K	585	ILE	4.5
1	C	587	ARG	4.4
1	E	80	GLY	4.4
1	F	588	ALA	4.3
1	D	620	ILE	4.3
1	G	620	ILE	4.1
1	I	584	ASN	4.1
1	F	587	ARG	4.1
1	G	621	SER	3.9
1	E	587	ARG	3.7
1	C	620	ILE	3.6
1	C	585	ILE	3.6
1	A	175	ARG	3.6
1	L	531	HIS	3.5
1	K	619	LEU	3.4
1	C	590	GLU	3.4
1	E	79	THR	3.3
1	E	315	PRO	3.3
1	H	315	PRO	3.3
1	K	587	ARG	3.3
1	B	11	ASP	3.2
1	C	439	LEU	3.2
1	E	586	SER	3.2
1	B	621	SER	3.2
1	C	315	PRO	3.2
1	E	416	LEU	3.1
1	E	531	HIS	3.1
1	C	533	ILE	3.1
1	I	589	ARG	3.1
1	K	79	THR	3.1
1	E	5	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	619	LEU	3.1
1	J	620	ILE	3.1
1	I	79	THR	3.0
1	D	12	GLY	3.0
1	H	620	ILE	3.0
1	E	316	TYR	3.0
1	I	316	TYR	3.0
1	K	439	LEU	3.0
1	A	617	PHE	3.0
1	A	16	ARG	3.0
1	F	620	ILE	3.0
1	E	589	ARG	2.9
1	E	193	ASN	2.9
1	B	620	ILE	2.9
1	I	409	ILE	2.8
1	L	585	ILE	2.8
1	C	408	TYR	2.8
1	K	531	HIS	2.8
1	F	530	ALA	2.8
1	A	12	GLY	2.8
1	H	61	HIS	2.8
1	A	620	ILE	2.8
1	C	5	PHE	2.8
1	E	412	ILE	2.7
1	C	619	LEU	2.7
1	E	530	ALA	2.7
1	E	81	ASN	2.7
1	C	290	GLU	2.7
1	B	532	GLY	2.6
1	C	589	ARG	2.6
1	K	193	ASN	2.6
1	F	15	ASP	2.6
1	C	6	LYS	2.6
1	I	80	GLY	2.6
1	F	494	VAL	2.6
1	F	318	GLN	2.6
1	F	531	HIS	2.6
1	H	8	ILE	2.6
1	L	588	ALA	2.6
1	C	440	LYS	2.6
1	L	530	ALA	2.5
1	L	438	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	60	SER	2.5
1	E	6	LYS	2.5
1	F	585	ILE	2.5
1	I	439	LEU	2.5
1	G	617	PHE	2.5
1	K	586	SER	2.5
1	B	531	HIS	2.4
1	A	301	TRP	2.4
1	L	587	ARG	2.4
1	I	583	VAL	2.4
1	K	194	GLY	2.4
1	H	318	GLN	2.4
1	F	589	ARG	2.4
1	F	532	GLY	2.4
1	C	412	ILE	2.4
1	H	361	VAL	2.3
1	E	417	ILE	2.3
1	C	316	TYR	2.3
1	H	316	TYR	2.3
1	E	584	ASN	2.3
1	L	532	GLY	2.3
1	L	389	GLN	2.3
1	K	314	ILE	2.3
1	E	4	VAL	2.3
1	H	273	ARG	2.3
1	B	588	ALA	2.2
1	C	586	SER	2.2
1	K	589	ARG	2.2
1	L	494	VAL	2.2
1	K	6	LYS	2.2
1	C	215	ASP	2.2
1	I	315	PRO	2.2
1	I	6	LYS	2.2
1	C	618	LEU	2.2
1	D	47	LEU	2.2
1	G	416	LEU	2.2
1	F	314	ILE	2.2
1	F	586	SER	2.2
1	L	111	THR	2.1
1	L	618	LEU	2.1
1	C	31	ILE	2.1
1	K	196	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	617	PHE	2.1
1	H	9	ALA	2.1
1	J	617	PHE	2.1
1	C	530	ALA	2.1
1	H	584	ASN	2.1
1	L	584	ASN	2.1
1	D	75	THR	2.1
1	I	26	ASP	2.1
1	K	315	PRO	2.1
1	E	440	LYS	2.1
1	I	436	GLN	2.0
1	I	619	LEU	2.0
1	E	314	ILE	2.0
1	J	75	THR	2.0
1	C	197	LEU	2.0
1	I	440	LYS	2.0
1	F	83	THR	2.0
1	I	586	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 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.