Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:14 pm BST

PDB ID	:	4ZOQ
Title	:	Crystal Structure of a Lanthipeptide Protease
Authors	:	Dong, S.H.; Nair, S.K.
Deposited on	:	2015-05-06
Resolution	:	2.35 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 following versions of software and data (see references ⓘ) were used in the production of this report:

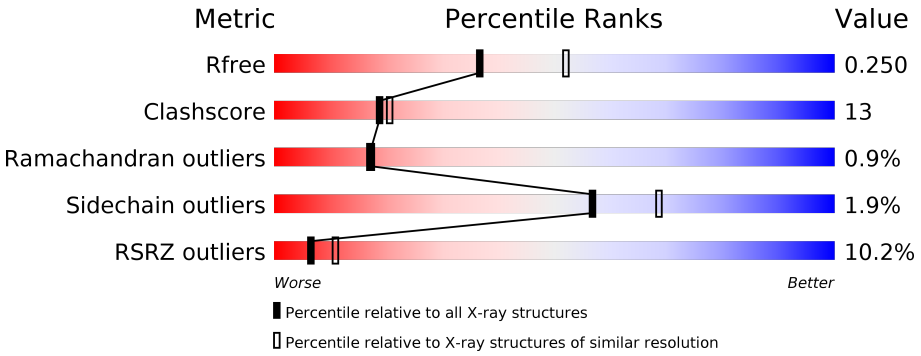
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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 <=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	100	8% 39% 22% 39%
1	B	100	12% 50% 10% 40%
1	C	100	11% 41% 18% • 40%
1	D	100	29% 31% 28% • 40%
1	E	100	43% 30% 25% 6% 39%
1	F	100	38% 25% 34% • 38%

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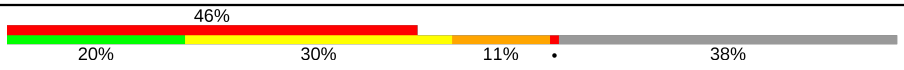
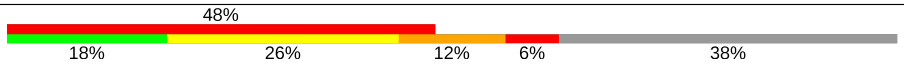
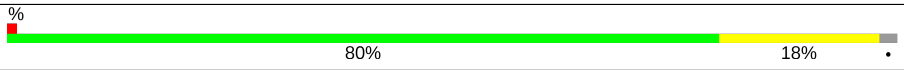
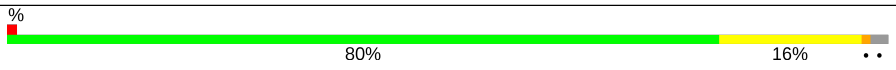
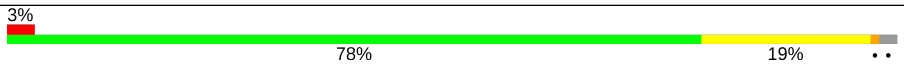
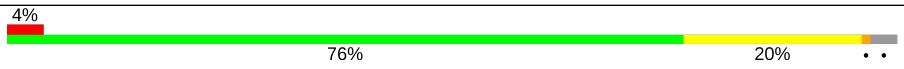
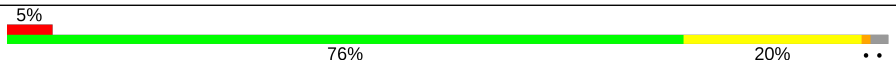
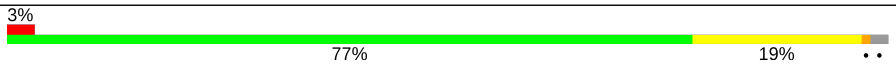
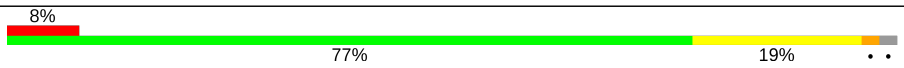
Mol	Chain	Length	Quality of chain
1	G	100	
1	H	100	
2	I	343	
2	J	343	
2	K	343	
2	L	343	
2	M	343	
2	N	343	
2	O	343	
2	P	343	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25562 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 Intracellular serine protease.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	61	Total	C	N	O	0	0	0
			486	314	79	93			
1	B	60	Total	C	N	O	0	0	0
			477	309	78	90			
1	C	60	Total	C	N	O	0	0	0
			477	309	78	90			
1	D	60	Total	C	N	O	0	0	0
			473	306	77	90			
1	E	61	Total	C	N	O	0	0	0
			478	309	78	91			
1	F	62	Total	C	N	O	0	0	0
			487	314	79	94			
1	G	62	Total	C	N	O	0	0	0
			483	312	79	92			
1	H	62	Total	C	N	O	0	0	0
			487	315	80	92			

- Molecule 2 is a protein called Intracellular serine protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	337	Total	C	N	O	S	0	0	0
			2586	1623	451	502	10			
2	J	337	Total	C	N	O	S	0	0	0
			2586	1623	451	502	10			
2	K	335	Total	C	N	O	S	0	0	0
			2571	1612	449	500	10			
2	L	337	Total	C	N	O	S	0	0	0
			2586	1623	451	502	10			
2	M	333	Total	C	N	O	S	0	0	0
			2557	1607	447	494	9			
2	N	335	Total	C	N	O	S	0	0	0
			2571	1612	449	500	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	335	Total	C	N	O	S	0	0	0
			2571	1612	449	500	10			
2	P	337	Total	C	N	O	S	0	0	0
			2586	1623	451	502	10			

- Molecule 3 is water.

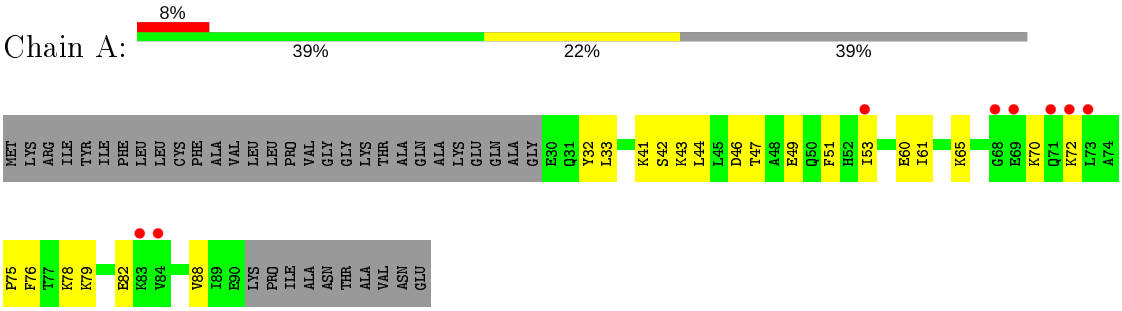
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	I	176	Total	O	0	0
			176	176		
3	B	20	Total	O	0	0
			20	20		
3	J	150	Total	O	0	0
			150	150		
3	C	21	Total	O	0	0
			21	21		
3	K	164	Total	O	0	0
			164	164		
3	D	4	Total	O	0	0
			4	4		
3	L	98	Total	O	0	0
			98	98		
3	E	9	Total	O	0	0
			9	9		
3	M	109	Total	O	0	0
			109	109		
3	F	3	Total	O	0	0
			3	3		
3	N	113	Total	O	0	0
			113	113		
3	G	5	Total	O	0	0
			5	5		
3	O	110	Total	O	0	0
			110	110		
3	H	3	Total	O	0	0
			3	3		
3	P	97	Total	O	0	0
			97	97		

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 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.

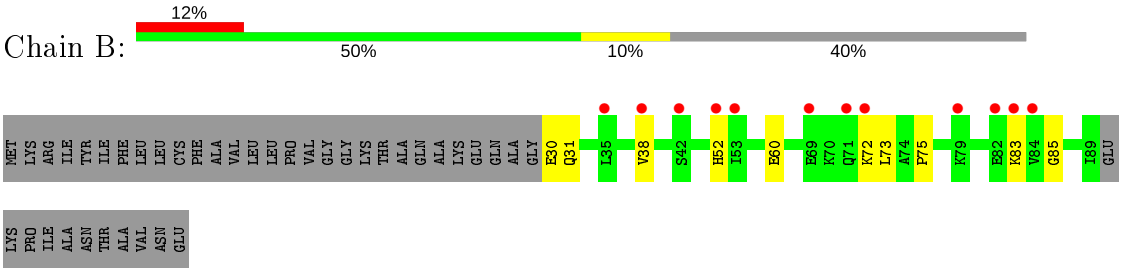
- Molecule 1: Intracellular serine protease

Chain A:



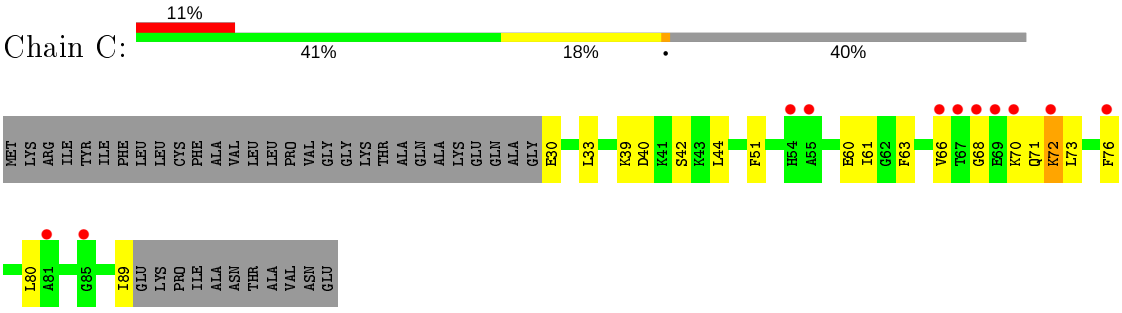
- Molecule 1: Intracellular serine protease

Chain B:



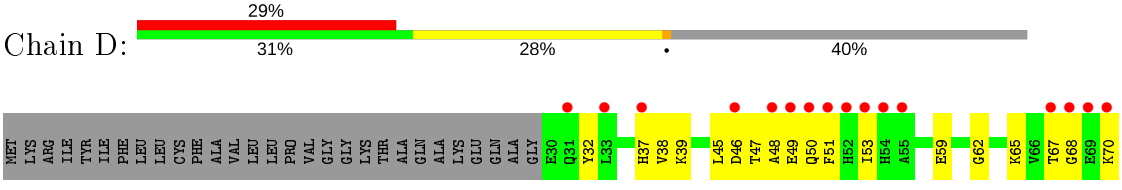
- Molecule 1: Intracellular serine protease

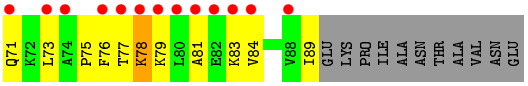
Chain C:



- Molecule 1: Intracellular serine protease

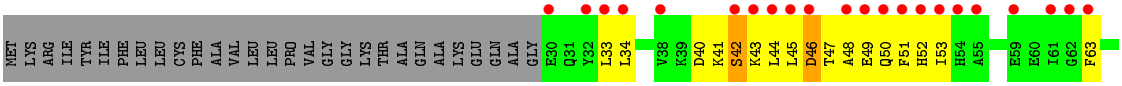
Chain D:

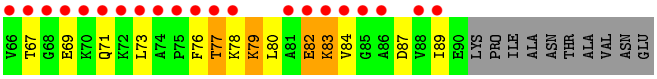




• Molecule 1: Intracellular serine protease

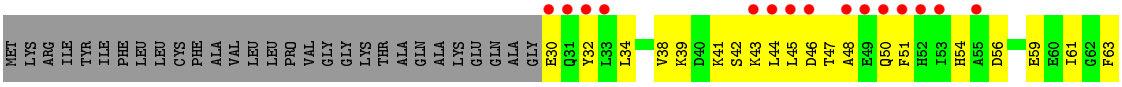
Chain E:

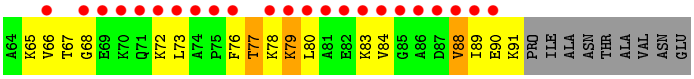




• Molecule 1: Intracellular serine protease

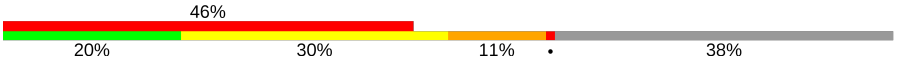
Chain F:

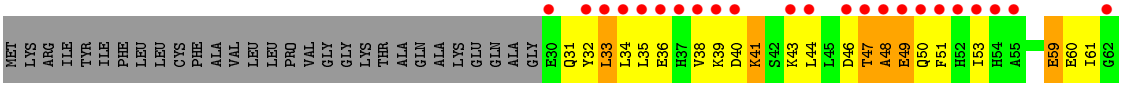


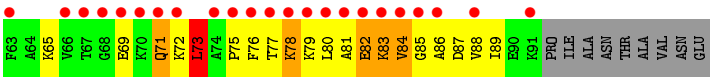


• Molecule 1: Intracellular serine protease

Chain G:

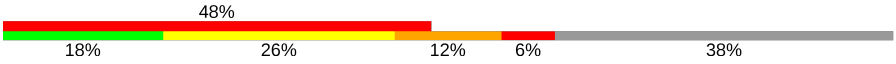


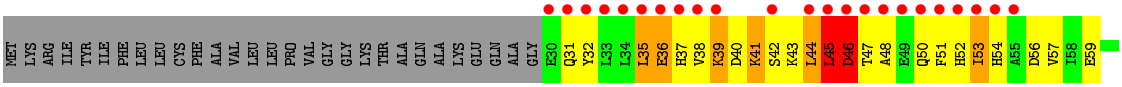


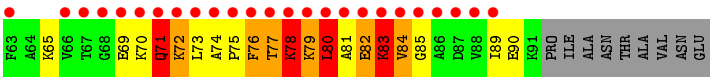


• Molecule 1: Intracellular serine protease

Chain H:





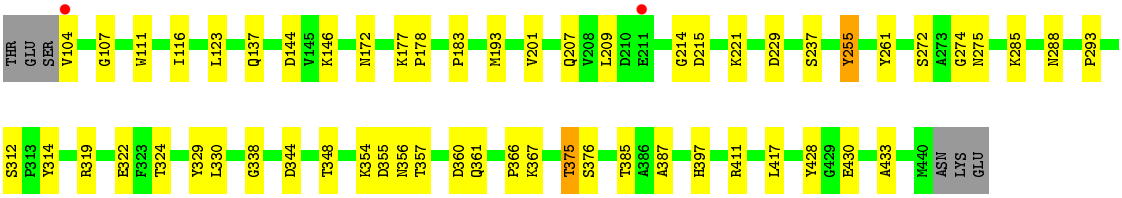


• Molecule 2: Intracellular serine protease

Chain I:

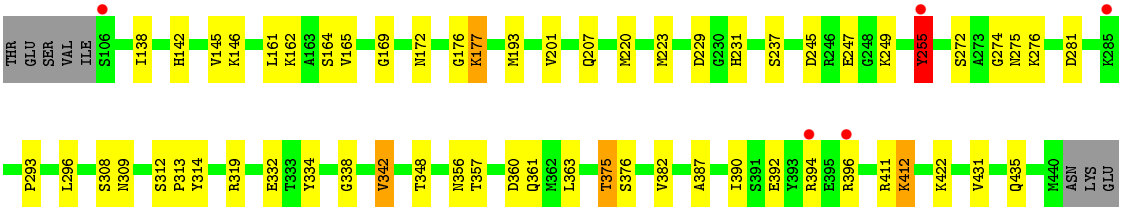
• Molecule 2: Intracellular serine protease

Chain J:



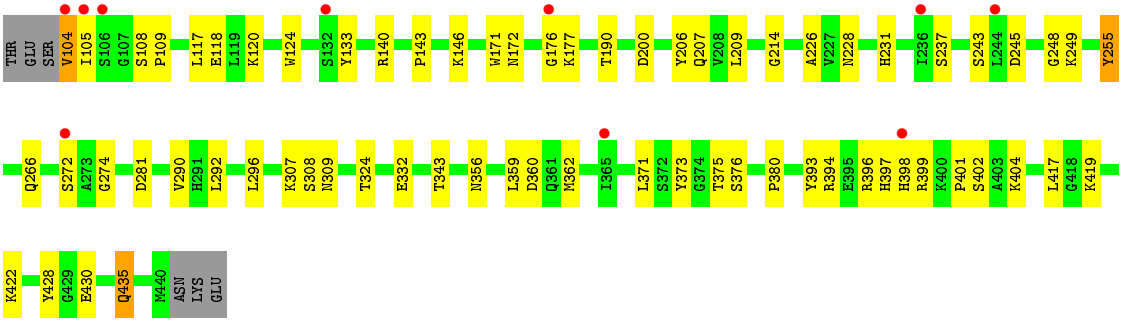
• Molecule 2: Intracellular serine protease

Chain K:



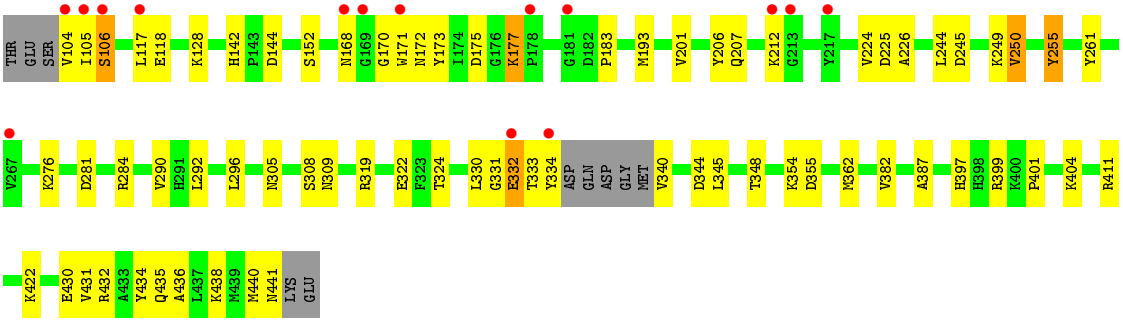
• Molecule 2: Intracellular serine protease

Chain L:



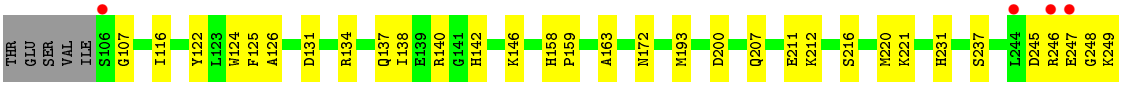
• Molecule 2: Intracellular serine protease

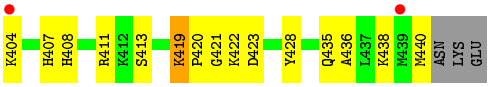
Chain M:



• Molecule 2: Intracellular serine protease

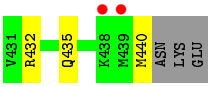
Chain N:





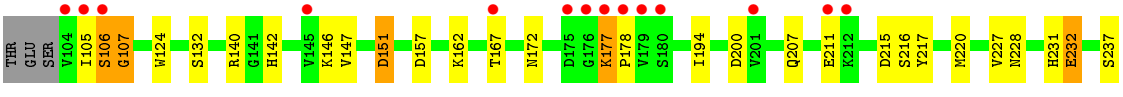
• Molecule 2: Intracellular serine protease

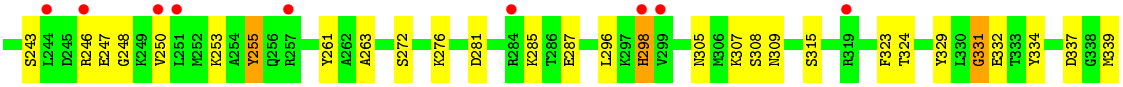
Chain O:

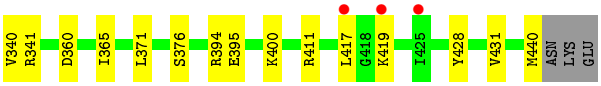


• Molecule 2: Intracellular serine protease

Chain P:






V340
R341
D360
I365
L371
S376
R394
E395
K400
R411
L417
G418
K419
I425
Y428
V431
M440
ASN
LYS
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.04Å 112.78Å 114.77Å 82.17° 89.68° 82.85°	Depositor
Resolution (Å)	38.03 – 2.35 38.54 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.03-2.35) 98.5 (38.54-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.200 , 0.250 0.201 , 0.250	Depositor DCC
R_{free} test set	7186 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25562	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.49	0/493	0.77	0/661
1	B	0.43	0/484	0.64	0/649
1	C	0.45	0/484	0.80	1/649 (0.2%)
1	D	0.48	0/480	0.80	1/645 (0.2%)
1	E	0.54	0/485	1.07	1/652 (0.2%)
1	F	0.62	0/494	0.93	1/664 (0.2%)
1	G	0.56	0/490	1.12	4/659 (0.6%)
1	H	0.85	0/494	1.82	15/663 (2.3%)
2	I	0.51	0/2639	0.64	0/3576
2	J	0.50	0/2639	0.65	2/3576 (0.1%)
2	K	0.55	1/2624 (0.0%)	0.70	2/3555 (0.1%)
2	L	0.47	0/2639	0.66	1/3576 (0.0%)
2	M	0.48	0/2609	0.68	1/3535 (0.0%)
2	N	0.47	0/2624	0.66	1/3555 (0.0%)
2	O	0.47	0/2624	0.66	0/3555
2	P	0.47	0/2639	0.69	2/3576 (0.1%)
All	All	0.50	1/24941 (0.0%)	0.74	32/33746 (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	D	0	1
1	E	0	4
1	G	0	1
1	H	0	6
2	L	0	1
2	M	0	1
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	255	TYR	CD2-CE2	-5.10	1.31	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	80	LEU	CA-CB-CG	14.99	149.77	115.30
1	H	83	LYS	N-CA-C	11.79	142.84	111.00
1	H	44	LEU	CB-CG-CD2	-10.56	93.04	111.00
1	H	71	GLN	N-CA-C	9.38	136.33	111.00
1	H	45	LEU	CA-CB-CG	-9.10	94.36	115.30
1	H	78	LYS	CA-CB-CG	7.99	130.98	113.40
1	H	83	LYS	C-N-CA	7.95	141.57	121.70
1	H	78	LYS	CB-CG-CD	7.11	130.08	111.60
1	H	35	LEU	CB-CG-CD1	-7.09	98.95	111.00
2	P	331	GLY	N-CA-C	-7.04	95.49	113.10
1	H	71	GLN	N-CA-CB	-6.50	98.89	110.60
1	H	83	LYS	CA-C-N	-6.49	102.93	117.20
2	M	331	GLY	N-CA-C	-6.35	97.22	113.10
1	G	83	LYS	CD-CE-NZ	6.09	125.70	111.70
2	J	107	GLY	N-CA-C	-6.06	97.95	113.10
1	G	73	LEU	CA-CB-CG	-5.92	101.69	115.30
1	G	84	VAL	CB-CA-C	-5.78	100.42	111.40
1	E	45	LEU	CA-CB-CG	5.71	128.42	115.30
2	J	397	HIS	N-CA-C	-5.69	95.64	111.00
1	H	37	HIS	N-CA-CB	5.66	120.79	110.60
2	N	248	GLY	N-CA-C	-5.58	99.15	113.10
1	D	68	GLY	N-CA-C	-5.58	99.16	113.10
1	H	70	LYS	C-N-CA	5.57	135.63	121.70
1	C	68	GLY	N-CA-C	-5.54	99.26	113.10
2	L	176	GLY	N-CA-C	-5.50	99.35	113.10
1	H	80	LEU	CB-CG-CD1	5.34	120.08	111.00
2	K	176	GLY	N-CA-C	-5.24	99.99	113.10
1	H	83	LYS	CB-CA-C	-5.22	99.97	110.40
2	P	107	GLY	N-CA-C	-5.17	100.17	113.10
1	G	33	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	F	88	VAL	C-N-CA	-5.06	109.06	121.70
2	K	255	TYR	CB-CG-CD2	-5.05	117.97	121.00

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	79	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	E	46	ASP	Peptide
1	E	77	THR	Peptide
1	E	79	LYS	Peptide
1	E	83	LYS	Peptide
1	G	71	GLN	Peptide
1	H	36	GLU	Peptide
1	H	45	LEU	Peptide
1	H	46	ASP	Peptide
1	H	77	THR	Peptide
1	H	80	LEU	Peptide
1	H	82	GLU	Peptide
2	L	118	GLU	Peptide
2	M	106	SER	Peptide

5.2 Too-close contacts (i)

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	486	0	499	19	0
1	B	477	0	493	10	0
1	C	477	0	493	13	0
1	D	473	0	482	23	0
1	E	478	0	484	30	0
1	F	487	0	490	46	0
1	G	483	0	486	46	0
1	H	487	0	497	57	0
2	I	2586	0	2557	42	0
2	J	2586	0	2557	39	0
2	K	2571	0	2537	49	0
2	L	2586	0	2557	49	0
2	M	2557	0	2534	55	1
2	N	2571	0	2537	63	0
2	O	2571	0	2537	62	1
2	P	2586	0	2557	60	0
3	A	18	0	0	8	0
3	B	20	0	0	5	0
3	C	21	0	0	3	0
3	D	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	9	0	0	0	0
3	F	3	0	0	3	0
3	G	5	0	0	3	0
3	H	3	0	0	2	0
3	I	176	0	0	11	0
3	J	150	0	0	13	1
3	K	164	0	0	14	0
3	L	98	0	0	8	0
3	M	109	0	0	18	0
3	N	113	0	0	15	0
3	O	110	0	0	12	1
3	P	97	0	0	13	0
All	All	25562	0	24297	638	2

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 13.

All (638) 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:G:33:LEU:HD11	1:G:86:ALA:HB1	1.31	1.09
1:H:41:LYS:HG3	1:H:45:LEU:HD13	1.30	1.08
1:B:30:GLU:N	3:B:201:HOH:O	1.89	1.02
2:L:272:SER:HB2	2:L:375:THR:HG23	1.40	1.00
2:J:274:GLY:H	2:J:375:THR:HG21	1.27	0.99
1:H:80:LEU:O	1:H:82:GLU:N	1.99	0.96
2:O:272:SER:HB2	2:O:375:THR:HG23	1.47	0.96
1:H:35:LEU:HD11	1:H:44:LEU:HD21	1.48	0.95
2:O:341:ARG:NH1	3:O:502:HOH:O	2.02	0.90
1:G:87:ASP:OD2	3:G:501:HOH:O	1.88	0.90
2:K:274:GLY:H	2:K:375:THR:HG21	1.34	0.90
2:M:183:PRO:O	2:M:354:LYS:NZ	2.06	0.89
2:N:211:GLU:O	3:N:501:HOH:O	1.90	0.88
2:N:246:ARG:NH1	2:N:247:GLU:OE2	2.07	0.86
1:G:77:THR:HB	1:G:88:VAL:HG21	1.55	0.86
1:G:83:LYS:HG3	1:G:84:VAL:HG13	1.58	0.86
1:F:79:LYS:HE2	1:F:80:LEU:HG	1.58	0.85
2:J:272:SER:HB2	2:J:375:THR:HG22	1.57	0.85
2:P:395:GLU:OE1	3:P:502:HOH:O	1.96	0.83
2:P:315:SER:O	3:P:501:HOH:O	1.95	0.83
2:O:274:GLY:H	2:O:375:THR:HG21	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:104:VAL:HG22	2:M:105:ILE:HD12	1.61	0.82
2:L:417:LEU:O	3:L:502:HOH:O	1.96	0.82
1:H:71:GLN:HG3	1:H:72:LYS:HG3	1.62	0.82
2:O:336:GLN:HE22	2:O:341:ARG:HE	1.28	0.82
1:G:46:ASP:N	3:G:502:HOH:O	2.07	0.81
2:I:157:ASP:O	2:I:352:LYS:NZ	2.12	0.81
2:M:355:ASP:O	3:M:501:HOH:O	1.98	0.81
1:B:83:LYS:NZ	3:B:205:HOH:O	2.12	0.81
2:O:336:GLN:NE2	2:O:341:ARG:HE	1.78	0.81
2:K:276:LYS:NZ	3:K:505:HOH:O	2.14	0.81
1:H:41:LYS:O	1:H:43:LYS:N	2.14	0.81
2:N:271:SER:OG	3:N:503:HOH:O	1.99	0.80
2:N:421:GLY:O	3:N:502:HOH:O	1.97	0.80
2:J:361:GLN:NE2	3:J:505:HOH:O	2.15	0.80
2:N:255:TYR:HB3	2:N:296:LEU:HD11	1.64	0.80
2:I:419:LYS:O	3:I:501:HOH:O	1.99	0.80
2:O:332:GLU:N	3:O:505:HOH:O	2.15	0.80
1:B:85:GLY:O	3:B:202:HOH:O	2.00	0.79
1:H:76:PHE:HB3	1:H:79:LYS:HG2	1.64	0.79
2:P:281:ASP:OD1	3:P:503:HOH:O	1.99	0.79
2:L:281:ASP:OD2	3:L:503:HOH:O	2.01	0.78
1:F:76:PHE:O	1:F:79:LYS:N	2.16	0.78
2:I:276:LYS:NZ	3:I:503:HOH:O	2.16	0.78
2:K:332:GLU:O	3:K:501:HOH:O	2.02	0.78
2:I:398:HIS:CE1	2:L:171:TRP:CG	2.71	0.78
1:F:77:THR:HG21	1:F:88:VAL:HG21	1.66	0.77
2:P:232:GLU:OE2	2:P:394:ARG:NH2	2.17	0.77
2:J:144:ASP:O	3:J:502:HOH:O	2.02	0.77
1:H:81:ALA:HA	1:H:83:LYS:HE2	1.67	0.77
2:K:275:ASN:OD1	2:K:375:THR:HB	1.85	0.77
1:F:73:LEU:HA	1:F:76:PHE:HB3	1.68	0.76
1:H:71:GLN:HG3	1:H:72:LYS:CG	2.15	0.76
2:L:343:THR:OG1	3:L:504:HOH:O	2.03	0.76
1:H:78:LYS:HG3	1:H:80:LEU:HB3	1.66	0.75
2:K:281:ASP:OD2	3:K:502:HOH:O	2.05	0.75
1:G:36:GLU:CD	1:G:85:GLY:HA3	2.07	0.75
2:J:104:VAL:N	3:J:510:HOH:O	2.19	0.75
2:L:402:SER:OG	3:L:501:HOH:O	1.91	0.74
2:N:408:HIS:ND1	3:N:505:HOH:O	2.19	0.74
1:F:73:LEU:HA	1:F:76:PHE:CB	2.17	0.74
2:J:215:ASP:OD2	3:J:503:HOH:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:396:ARG:NH2	3:N:506:HOH:O	2.21	0.74
1:E:49:GLU:HA	1:E:52:HIS:HA	1.68	0.73
1:E:79:LYS:NZ	1:E:82:GLU:O	2.21	0.73
1:A:70:LYS:O	3:A:201:HOH:O	2.06	0.73
2:J:288:ASN:OD1	3:J:504:HOH:O	2.07	0.73
1:F:42:SER:O	3:F:201:HOH:O	2.06	0.72
2:K:162:LYS:O	3:K:503:HOH:O	2.07	0.72
2:L:274:GLY:H	2:L:375:THR:HG21	1.54	0.72
1:E:47:THR:HA	1:E:50:GLN:HE21	1.54	0.72
1:E:42:SER:OG	1:E:43:LYS:N	2.23	0.72
1:F:79:LYS:HG3	1:F:80:LEU:H	1.53	0.72
2:O:419:LYS:O	3:O:503:HOH:O	2.08	0.72
2:P:167:THR:OG1	3:P:504:HOH:O	2.06	0.72
2:J:272:SER:HB2	2:J:375:THR:CG2	2.18	0.71
2:I:417:LEU:O	3:I:501:HOH:O	2.07	0.71
2:N:216:SER:HB3	2:N:255:TYR:HE1	1.55	0.71
1:H:78:LYS:HG3	1:H:80:LEU:CB	2.21	0.70
2:J:275:ASN:OD1	2:J:375:THR:HB	1.91	0.70
2:K:142:HIS:ND1	3:K:508:HOH:O	2.24	0.70
2:L:237:SER:HB3	2:L:376:SER:HB2	1.73	0.70
2:P:227:VAL:O	3:P:506:HOH:O	2.09	0.70
1:H:80:LEU:O	1:H:83:LYS:N	2.24	0.69
2:K:272:SER:HB2	2:K:375:THR:HG22	1.73	0.69
1:E:40:ASP:OD2	1:E:84:VAL:HG21	1.91	0.69
2:N:305:ASN:HD22	2:N:324:THR:HG23	1.58	0.69
1:B:60:GLU:OE1	3:B:204:HOH:O	2.11	0.69
2:I:245:ASP:OD1	3:I:502:HOH:O	2.11	0.69
2:N:411:ARG:HD2	2:N:428:TYR:CE1	2.27	0.69
1:H:45:LEU:HD11	1:H:57:VAL:HG21	1.74	0.68
1:H:48:ALA:HA	1:H:51:PHE:HD2	1.58	0.68
2:J:183:PRO:HD2	3:J:577:HOH:O	1.93	0.68
2:O:160:ASP:OD1	3:O:504:HOH:O	2.11	0.68
2:J:221:LYS:NZ	3:J:501:HOH:O	1.84	0.68
2:K:247:GLU:OE1	3:K:504:HOH:O	2.11	0.68
2:M:276:LYS:NZ	3:M:505:HOH:O	2.26	0.68
2:P:440:MET:O	3:P:507:HOH:O	2.11	0.67
1:E:46:ASP:OD1	1:E:50:GLN:N	2.27	0.67
2:K:272:SER:HB2	2:K:375:THR:CG2	2.25	0.67
2:L:419:LYS:O	3:L:502:HOH:O	2.11	0.67
2:K:165:VAL:O	3:K:503:HOH:O	2.13	0.67
2:M:249:LYS:HD2	3:M:537:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:332:GLU:OE1	3:N:504:HOH:O	2.13	0.66
2:P:337:ASP:O	3:P:508:HOH:O	2.12	0.66
1:C:71:GLN:O	1:C:73:LEU:N	2.26	0.66
2:M:332:GLU:O	2:M:333:THR:HG23	1.95	0.66
2:O:336:GLN:HE22	2:O:341:ARG:NE	1.94	0.66
2:P:142:HIS:CE1	2:P:395:GLU:HG3	2.31	0.66
1:A:42:SER:OG	3:A:202:HOH:O	2.12	0.66
2:M:183:PRO:HD2	3:M:527:HOH:O	1.96	0.66
1:H:56:ASP:OD1	3:H:201:HOH:O	2.13	0.66
1:F:90:GLU:HG2	1:F:91:LYS:H	1.61	0.65
2:O:331:GLY:O	2:O:333:THR:N	2.30	0.65
1:C:42:SER:OG	3:C:201:HOH:O	2.14	0.65
1:E:46:ASP:OD1	1:E:49:GLU:N	2.30	0.65
1:F:90:GLU:HG2	1:F:91:LYS:N	2.11	0.65
2:P:142:HIS:NE2	2:P:395:GLU:HG3	2.12	0.65
2:K:138:ILE:O	3:K:506:HOH:O	2.15	0.64
2:L:104:VAL:HG22	2:L:105:ILE:HD12	1.80	0.64
2:P:287:GLU:OE2	3:P:509:HOH:O	2.15	0.64
1:A:46:ASP:OD1	3:A:203:HOH:O	2.15	0.63
2:P:337:ASP:HB3	2:P:339:MET:H	1.62	0.63
2:I:412:LYS:HB2	2:I:439:MET:HE1	1.79	0.63
2:J:201:VAL:HG21	2:J:387:ALA:HB1	1.81	0.63
1:G:73:LEU:HD23	1:G:79:LYS:HD3	1.81	0.63
1:C:30:GLU:N	3:C:204:HOH:O	2.31	0.63
1:H:69:GLU:HG3	1:H:71:GLN:HB3	1.81	0.63
2:M:344:ASP:OD1	3:M:502:HOH:O	2.15	0.63
1:C:63:PHE:CD2	2:K:220:MET:HE1	2.34	0.62
1:H:31:GLN:HB3	1:H:89:ILE:O	1.98	0.62
2:N:142:HIS:CD2	2:N:391:SER:HB3	2.34	0.62
1:F:43:LYS:HD3	1:F:83:LYS:HE2	1.81	0.62
1:F:56:ASP:OD2	2:N:221:LYS:NZ	2.30	0.61
2:M:332:GLU:HG3	2:M:332:GLU:O	2.00	0.61
2:K:237:SER:HB3	2:K:376:SER:HB2	1.82	0.61
2:M:193:MET:HE1	2:M:348:THR:HA	1.81	0.61
1:G:73:LEU:HG	1:G:75:PRO:HD2	1.83	0.61
2:P:215:ASP:OD2	2:P:217:TYR:HB3	2.01	0.61
1:H:41:LYS:HZ2	1:H:57:VAL:HB	1.65	0.61
2:O:106:SER:N	3:O:515:HOH:O	2.33	0.61
1:H:80:LEU:HD22	1:H:83:LYS:HD3	1.83	0.60
2:I:104:VAL:N	3:I:508:HOH:O	2.34	0.60
2:K:342:VAL:HG21	2:K:363:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:435:GLN:OE1	2:L:435:GLN:HA	2.01	0.60
2:J:355:ASP:HA	2:J:367:LYS:HE2	1.84	0.60
1:H:78:LYS:NZ	1:H:80:LEU:HB2	2.15	0.60
2:K:164:SER:OG	3:K:507:HOH:O	2.16	0.60
1:D:53:ILE:HG23	1:D:67:THR:O	2.02	0.60
2:I:249:LYS:O	3:I:504:HOH:O	2.16	0.60
2:K:255:TYR:CZ	2:K:293:PRO:HB3	2.36	0.60
2:N:116:ILE:HD12	2:N:366:PRO:HG3	1.84	0.60
1:G:38:VAL:HG21	1:G:59:GLU:O	2.01	0.59
1:H:69:GLU:HG3	1:H:71:GLN:CB	2.31	0.59
1:G:79:LYS:HA	1:G:82:GLU:OE2	2.01	0.59
2:L:117:LEU:O	2:L:120:LYS:HG3	2.02	0.59
2:N:131:ASP:OD2	2:N:134:ARG:HD2	2.01	0.59
2:J:319:ARG:NE	3:J:517:HOH:O	2.34	0.59
2:K:255:TYR:CD2	2:K:296:LEU:HD11	2.37	0.59
2:J:146:LYS:NZ	2:J:229:ASP:O	2.33	0.59
1:D:71:GLN:O	1:D:75:PRO:HD3	2.03	0.59
1:H:83:LYS:HD2	1:H:85:GLY:HA2	1.84	0.59
2:M:401:PRO:HG2	3:M:549:HOH:O	2.02	0.59
2:L:266:GLN:OE1	3:L:505:HOH:O	2.17	0.59
1:F:77:THR:HA	1:F:79:LYS:HG2	1.85	0.59
2:K:274:GLY:N	2:K:375:THR:HG21	2.13	0.59
1:D:37:HIS:CD2	1:D:39:LYS:H	2.20	0.59
1:H:41:LYS:HG3	1:H:45:LEU:CD1	2.20	0.59
1:F:72:LYS:O	1:F:76:PHE:HB2	2.02	0.59
2:J:417:LEU:O	3:J:506:HOH:O	2.16	0.59
2:L:172:ASN:HA	2:L:207:GLN:HB3	1.84	0.59
2:P:255:TYR:HB3	2:P:296:LEU:HD11	1.84	0.58
2:M:334:TYR:HA	3:M:540:HOH:O	2.02	0.58
2:O:109:PRO:HD2	2:O:120:LYS:HE3	1.84	0.58
2:O:336:GLN:NE2	2:O:341:ARG:NE	2.51	0.58
1:E:52:HIS:O	1:E:53:ILE:HD13	2.03	0.58
2:M:340:VAL:N	3:M:510:HOH:O	2.36	0.58
1:E:69:GLU:HG2	1:E:71:GLN:H	1.67	0.58
2:N:342:VAL:HG21	2:N:363:LEU:HD11	1.85	0.58
2:I:357:THR:O	2:I:361:GLN:HG3	2.03	0.58
1:A:43:LYS:HG3	3:A:202:HOH:O	2.04	0.58
2:N:422:LYS:HG3	2:N:428:TYR:CD1	2.39	0.58
1:F:79:LYS:HE2	1:F:80:LEU:CG	2.32	0.58
2:I:177:LYS:HG3	2:I:178:PRO:HD2	1.86	0.58
2:O:274:GLY:N	2:O:375:THR:HG21	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:LYS:CG	1:F:80:LEU:H	2.17	0.57
1:G:35:LEU:HD12	1:G:36:GLU:H	1.69	0.57
1:G:43:LYS:O	1:G:83:LYS:HE2	2.05	0.57
2:M:152:SER:HB2	3:M:527:HOH:O	2.03	0.57
2:P:281:ASP:O	2:P:285:LYS:HG2	2.04	0.57
2:N:419:LYS:HG2	2:N:421:GLY:H	1.70	0.57
1:A:51:PHE:O	1:A:72:LYS:HE3	2.05	0.57
2:K:357:THR:O	2:K:361:GLN:HG2	2.05	0.57
1:G:82:GLU:N	1:G:82:GLU:OE2	2.38	0.57
1:H:50:GLN:O	1:H:50:GLN:HG2	2.03	0.57
2:I:291:HIS:NE2	3:I:506:HOH:O	2.33	0.57
2:K:392:GLU:OE2	2:K:396:ARG:NH2	2.38	0.57
2:M:441:ASN:HB3	3:M:542:HOH:O	2.05	0.57
2:O:255:TYR:HB3	2:O:296:LEU:HD21	1.87	0.57
1:D:83:LYS:HG2	1:D:84:VAL:HG12	1.87	0.57
2:I:398:HIS:CE1	2:L:171:TRP:CD1	2.93	0.57
2:I:201:VAL:HG11	2:I:387:ALA:HB1	1.86	0.57
2:N:411:ARG:NH1	3:N:505:HOH:O	2.38	0.57
1:G:69:GLU:OE1	1:G:71:GLN:HG3	2.05	0.56
1:A:79:LYS:HA	1:A:82:GLU:HG3	1.87	0.56
1:B:72:LYS:C	1:B:75:PRO:HD2	2.26	0.56
1:F:44:LEU:HD12	1:F:79:LYS:NZ	2.20	0.56
1:G:76:PHE:HD1	1:G:79:LYS:HE2	1.69	0.56
2:O:237:SER:HB3	2:O:376:SER:HB2	1.86	0.56
1:D:37:HIS:HD2	1:D:39:LYS:H	1.54	0.56
1:D:49:GLU:HG2	1:D:49:GLU:O	2.05	0.56
2:K:145:VAL:HG22	2:K:394:ARG:HH11	1.70	0.56
2:N:255:TYR:CE2	2:N:293:PRO:HB3	2.40	0.56
1:D:38:VAL:HG13	1:D:59:GLU:O	2.06	0.56
2:N:142:HIS:HD2	2:N:391:SER:HB3	1.70	0.56
2:J:137:GLN:O	2:J:137:GLN:HG2	2.05	0.56
2:L:356:ASN:HB2	2:L:360:ASP:OD2	2.06	0.55
2:J:338:GLY:O	3:J:509:HOH:O	2.18	0.55
1:F:44:LEU:HD12	1:F:79:LYS:HZ3	1.72	0.55
2:M:128:LYS:HE2	2:M:309:ASN:OD1	2.07	0.55
2:P:341:ARG:NE	3:P:505:HOH:O	2.07	0.55
1:A:78:LYS:NZ	3:A:207:HOH:O	2.37	0.55
1:E:46:ASP:HA	1:E:48:ALA:H	1.72	0.55
2:J:237:SER:HB3	2:J:376:SER:HB2	1.87	0.55
1:D:37:HIS:HD2	1:D:38:VAL:N	2.05	0.54
2:K:319:ARG:O	2:K:422:LYS:HE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:423:ASP:OD1	3:N:502:HOH:O	2.18	0.54
2:P:177:LYS:HB2	2:P:178:PRO:HD2	1.89	0.54
1:H:41:LYS:HD3	1:H:59:GLU:CD	2.28	0.54
1:E:34:LEU:HB2	1:E:63:PHE:CE1	2.42	0.54
1:F:61:ILE:O	2:N:257:ARG:NH1	2.41	0.54
2:J:255:TYR:CE2	2:J:293:PRO:HB3	2.43	0.54
1:G:47:THR:HA	1:G:50:GLN:OE1	2.07	0.54
2:N:305:ASN:ND2	2:N:324:THR:HG23	2.23	0.54
2:K:255:TYR:CE2	2:K:293:PRO:HB3	2.43	0.54
1:F:76:PHE:O	1:F:78:LYS:N	2.42	0.54
2:I:237:SER:HB3	2:I:376:SER:HB2	1.90	0.54
2:P:157:ASP:HA	2:P:162:LYS:HG2	1.90	0.54
2:L:274:GLY:N	2:L:375:THR:HG21	2.23	0.53
2:N:216:SER:HB3	2:N:255:TYR:CE1	2.41	0.53
1:G:73:LEU:CD2	1:G:79:LYS:HD3	2.38	0.53
1:H:41:LYS:NZ	1:H:57:VAL:HB	2.22	0.53
1:H:77:THR:O	1:H:78:LYS:HB2	2.08	0.53
2:O:142:HIS:CE1	2:P:105:ILE:HG13	2.44	0.53
2:P:246:ARG:HG3	2:P:247:GLU:HB2	1.90	0.53
2:J:274:GLY:N	2:J:375:THR:HG21	2.11	0.53
2:P:157:ASP:CG	2:P:162:LYS:HD2	2.29	0.53
1:G:60:GLU:OE1	1:G:60:GLU:N	2.38	0.53
2:L:140:ARG:HD3	2:L:200:ASP:OD2	2.08	0.53
1:G:78:LYS:O	1:G:78:LYS:HG3	2.09	0.53
1:F:45:LEU:N	3:F:201:HOH:O	2.42	0.53
2:O:275:ASN:ND2	3:O:507:HOH:O	2.19	0.53
2:P:246:ARG:CG	2:P:247:GLU:N	2.71	0.53
2:I:113:LEU:HD21	2:I:123:LEU:HD11	1.91	0.53
2:K:356:ASN:HB2	2:K:360:ASP:OD2	2.09	0.53
2:L:108:SER:HB2	2:L:109:PRO:HD2	1.91	0.53
1:F:47:THR:HG21	1:F:79:LYS:HE3	1.90	0.52
1:A:49:GLU:OE2	3:A:205:HOH:O	2.19	0.52
1:F:48:ALA:HA	1:F:76:PHE:CE1	2.44	0.52
1:E:89:ILE:HD11	2:M:250:VAL:HG12	1.91	0.52
2:J:209:LEU:HD23	2:J:214:GLY:HA3	1.90	0.52
2:M:104:VAL:HG22	2:M:105:ILE:N	2.25	0.52
1:G:51:PHE:CE1	1:G:79:LYS:NZ	2.74	0.52
2:I:333:THR:H	2:I:341:ARG:HH12	1.55	0.52
2:K:361:GLN:NE2	3:K:518:HOH:O	2.42	0.52
2:P:308:SER:O	2:P:309:ASN:HB2	2.09	0.52
1:F:34:LEU:HD11	2:N:257:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:LEU:HA	1:F:76:PHE:HB2	1.89	0.52
2:J:193:MET:HE1	2:J:348:THR:HA	1.91	0.52
2:J:172:ASN:HA	2:J:207:GLN:HB3	1.91	0.52
1:A:60:GLU:OE1	3:A:204:HOH:O	2.18	0.52
1:F:54:HIS:HB3	1:F:67:THR:OG1	2.10	0.52
1:G:48:ALA:O	1:G:53:ILE:HB	2.10	0.52
2:K:146:LYS:HB3	2:K:231:HIS:CD2	2.45	0.52
2:O:201:VAL:HG21	2:O:387:ALA:HB1	1.92	0.52
1:D:78:LYS:HA	1:D:81:ALA:HB3	1.92	0.51
2:O:332:GLU:HB3	2:O:335:ASP:OD1	2.09	0.51
1:D:73:LEU:O	1:D:77:THR:HG23	2.10	0.51
1:E:50:GLN:HG3	1:E:51:PHE:CD1	2.45	0.51
1:G:72:LYS:O	1:G:73:LEU:HB2	2.11	0.51
1:H:74:ALA:O	1:H:77:THR:HB	2.10	0.51
2:M:170:GLY:HA2	3:M:521:HOH:O	2.10	0.51
2:L:209:LEU:HD23	2:L:214:GLY:HA3	1.91	0.51
2:O:232:GLU:OE1	2:O:394:ARG:NH2	2.43	0.51
2:O:396:ARG:HH12	2:O:440:MET:HB3	1.75	0.51
2:P:246:ARG:HG2	2:P:247:GLU:N	2.26	0.51
1:E:82:GLU:CG	1:E:83:LYS:H	2.23	0.51
1:F:47:THR:CG2	1:F:79:LYS:HE3	2.40	0.51
1:H:32:TYR:CE1	1:H:65:LYS:HB2	2.46	0.51
2:K:172:ASN:HA	2:K:207:GLN:HB3	1.93	0.51
1:D:50:GLN:O	1:D:51:PHE:HD1	1.94	0.51
1:H:35:LEU:CD1	1:H:44:LEU:HD21	2.32	0.51
2:P:216:SER:O	2:P:220:MET:HG3	2.11	0.51
1:G:83:LYS:HG2	1:G:84:VAL:HG22	1.93	0.50
1:C:33:LEU:HD12	1:C:66:VAL:HG11	1.91	0.50
2:M:244:LEU:HD11	3:M:525:HOH:O	2.11	0.50
1:H:46:ASP:C	1:H:48:ALA:N	2.65	0.50
1:A:32:TYR:CE2	1:A:65:LYS:HB2	2.47	0.50
2:O:172:ASN:HA	2:O:207:GLN:HB3	1.94	0.50
2:O:177:LYS:HG2	2:O:178:PRO:O	2.11	0.50
2:O:393:TYR:OH	2:O:399:ARG:NH2	2.44	0.50
2:P:105:ILE:HG22	2:P:106:SER:O	2.12	0.50
1:G:73:LEU:HB3	1:G:76:PHE:HB2	1.92	0.50
2:I:337:ASP:OD2	2:I:341:ARG:NH2	2.44	0.50
2:J:183:PRO:O	2:J:354:LYS:NZ	2.39	0.50
2:J:319:ARG:NH1	3:J:523:HOH:O	2.44	0.50
2:M:201:VAL:HG21	2:M:387:ALA:HB1	1.94	0.50
1:G:80:LEU:HD22	1:G:83:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:245:ASP:O	2:O:249:LYS:HG3	2.11	0.50
2:O:331:GLY:HA2	3:O:506:HOH:O	2.11	0.50
2:I:307:LYS:NZ	3:I:516:HOH:O	2.41	0.50
2:O:142:HIS:NE2	2:O:395:GLU:OE2	2.45	0.50
1:F:39:LYS:HE3	1:F:39:LYS:HA	1.92	0.50
1:G:33:LEU:HD21	1:G:80:LEU:HD12	1.94	0.50
2:K:411:ARG:NH1	2:K:412:LYS:NZ	2.60	0.50
2:I:143:PRO:HD2	2:L:228:ASN:O	2.12	0.50
2:N:193:MET:HE3	3:N:559:HOH:O	2.11	0.50
2:N:394:ARG:HE	2:N:400:LYS:N	2.10	0.50
1:E:76:PHE:CZ	1:E:80:LEU:HD21	2.47	0.49
2:K:382:VAL:HG13	2:K:431:VAL:HG21	1.93	0.49
1:B:38:VAL:N	3:B:206:HOH:O	2.44	0.49
1:H:53:ILE:HG22	1:H:54:HIS:H	1.77	0.49
2:L:308:SER:OG	2:L:332:GLU:OE2	2.20	0.49
2:M:172:ASN:HA	2:M:207:GLN:HB3	1.93	0.49
2:O:146:LYS:HB3	2:O:231:HIS:CD2	2.46	0.49
1:E:79:LYS:C	1:E:82:GLU:H	2.14	0.49
2:I:322:GLU:HG3	3:I:512:HOH:O	2.10	0.49
2:M:255:TYR:HB3	2:M:296:LEU:HD11	1.94	0.49
2:M:432:ARG:NH2	2:M:435:GLN:HG2	2.26	0.49
2:O:149:LEU:HD11	2:O:194:ILE:CD1	2.43	0.49
1:G:61:ILE:HB	2:O:257:ARG:HG3	1.94	0.49
2:O:411:ARG:HD2	2:O:428:TYR:CE1	2.47	0.49
1:H:35:LEU:HB3	3:H:202:HOH:O	2.12	0.49
2:L:245:ASP:O	2:L:249:LYS:HG3	2.11	0.49
1:D:32:TYR:CE1	1:D:65:LYS:HB2	2.48	0.49
2:K:177:LYS:N	3:K:512:HOH:O	2.29	0.49
2:O:172:ASN:HB3	2:O:177:LYS:O	2.13	0.49
1:G:33:LEU:HD12	1:G:34:LEU:N	2.28	0.49
2:L:146:LYS:HB3	2:L:231:HIS:CD2	2.48	0.49
2:M:334:TYR:HB3	3:M:511:HOH:O	2.13	0.49
2:O:142:HIS:NE2	2:O:395:GLU:HG3	2.28	0.49
2:P:246:ARG:NH1	2:P:247:GLU:OE1	2.42	0.49
1:C:44:LEU:HD13	1:C:80:LEU:HD21	1.95	0.49
2:I:137:GLN:NE2	2:L:143:PRO:HB3	2.28	0.49
2:P:124:TRP:CD2	2:P:307:LYS:HE2	2.48	0.49
2:P:394:ARG:HH21	2:P:400:LYS:HE3	1.78	0.49
2:L:422:LYS:HD2	2:L:428:TYR:CE1	2.48	0.49
1:G:32:TYR:CE2	1:G:65:LYS:HB2	2.47	0.49
2:J:324:THR:HG22	2:J:430:GLU:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:THR:O	1:F:77:THR:HG22	2.13	0.49
1:G:73:LEU:HG	1:G:75:PRO:CD	2.43	0.49
1:H:72:LYS:C	1:H:73:LEU:HD12	2.33	0.49
2:M:104:VAL:HG22	2:M:105:ILE:H	1.76	0.49
1:H:90:GLU:H	2:P:247:GLU:CD	2.16	0.49
1:G:43:LYS:HB3	1:G:83:LYS:HD2	1.95	0.48
1:H:36:GLU:OE1	2:P:253:LYS:NZ	2.39	0.48
2:K:193:MET:HE1	2:K:348:THR:HA	1.95	0.48
2:L:397:HIS:O	2:L:399:ARG:N	2.46	0.48
2:P:360:ASP:HB3	2:P:365:ILE:HB	1.95	0.48
1:H:73:LEU:HA	1:H:76:PHE:CE1	2.47	0.48
2:M:290:VAL:HG13	2:M:292:LEU:HG	1.95	0.48
2:N:140:ARG:HD3	2:N:200:ASP:OD2	2.13	0.48
2:N:357:THR:O	2:N:361:GLN:HG3	2.13	0.48
2:O:335:ASP:N	3:O:506:HOH:O	2.17	0.48
2:P:237:SER:HB3	2:P:376:SER:HB2	1.96	0.48
2:P:172:ASN:HA	2:P:207:GLN:HB3	1.95	0.48
2:P:276:LYS:NZ	3:P:519:HOH:O	2.47	0.48
1:C:71:GLN:C	1:C:73:LEU:H	2.17	0.48
2:L:190:THR:HG23	2:L:380:PRO:HG3	1.94	0.48
2:M:104:VAL:HG22	2:M:105:ILE:CD1	2.40	0.48
1:F:38:VAL:HG13	1:F:59:GLU:O	2.13	0.48
1:F:63:PHE:CE2	2:N:220:MET:HE3	2.49	0.48
1:H:44:LEU:HG	1:H:45:LEU:HD12	1.96	0.48
2:N:107:GLY:HA2	3:N:539:HOH:O	2.14	0.48
2:N:422:LYS:CD	2:N:422:LYS:N	2.77	0.48
2:N:413:SER:HB2	2:N:435:GLN:HB3	1.95	0.48
1:D:45:LEU:O	1:D:48:ALA:HB3	2.14	0.47
1:E:76:PHE:CE1	1:E:80:LEU:HD11	2.49	0.47
2:I:329:TYR:CG	2:I:330:LEU:N	2.82	0.47
2:J:344:ASP:OD1	3:J:512:HOH:O	2.20	0.47
2:L:422:LYS:HD2	2:L:428:TYR:CZ	2.48	0.47
2:P:243:SER:O	2:P:248:GLY:HA3	2.14	0.47
2:I:190:THR:HG23	2:I:380:PRO:HG3	1.96	0.47
1:E:44:LEU:HG	1:E:80:LEU:HD23	1.97	0.47
2:P:107:GLY:HA3	2:P:132:SER:O	2.15	0.47
1:C:61:ILE:HA	3:C:205:HOH:O	2.14	0.47
1:E:82:GLU:HG3	1:E:83:LYS:H	1.80	0.47
2:O:254:ALA:O	2:O:257:ARG:HG2	2.13	0.47
2:P:211:GLU:CD	2:P:211:GLU:H	2.18	0.47
1:B:72:LYS:O	1:B:75:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:LYS:HA	1:G:82:GLU:CD	2.35	0.47
2:P:334:TYR:HB2	2:P:340:VAL:HG22	1.97	0.47
1:H:75:PRO:C	1:H:77:THR:H	2.18	0.47
2:L:371:LEU:HA	2:L:371:LEU:HD12	1.69	0.47
2:N:211:GLU:H	2:N:211:GLU:CD	2.18	0.47
2:P:140:ARG:HD3	2:P:200:ASP:OD2	2.15	0.47
2:P:419:LYS:HD3	2:P:419:LYS:HA	1.72	0.47
1:F:79:LYS:HG3	1:F:80:LEU:HG	1.97	0.47
1:F:89:ILE:HD12	2:N:247:GLU:HB2	1.97	0.47
1:H:35:LEU:HD21	1:H:44:LEU:CD2	2.45	0.47
2:I:209:LEU:HD23	2:I:214:GLY:HA3	1.97	0.47
2:K:313:PRO:HB2	2:K:334:TYR:CE2	2.50	0.47
1:G:46:ASP:O	1:G:50:GLN:HB2	2.15	0.47
1:H:78:LYS:HZ3	1:H:80:LEU:HB2	1.79	0.47
2:O:337:ASP:N	3:O:509:HOH:O	2.38	0.47
1:E:50:GLN:HG3	1:E:51:PHE:HD1	1.79	0.47
2:N:237:SER:HB3	2:N:376:SER:HB2	1.97	0.47
2:N:255:TYR:HE2	2:N:293:PRO:HB3	1.80	0.47
1:E:79:LYS:HG2	1:E:82:GLU:HA	1.97	0.46
2:K:223:MET:SD	2:K:255:TYR:CE2	3.08	0.46
1:G:43:LYS:C	3:G:502:HOH:O	2.52	0.46
2:L:308:SER:O	2:L:309:ASN:HB2	2.15	0.46
2:M:382:VAL:HG13	2:M:431:VAL:HG21	1.96	0.46
2:O:306:MET:HE2	2:O:310:ASN:HB2	1.97	0.46
1:D:77:THR:OG1	1:D:78:LYS:N	2.48	0.46
2:I:333:THR:H	2:I:341:ARG:NH1	2.13	0.46
2:K:412:LYS:HA	2:K:412:LYS:HD2	1.57	0.46
2:M:175:ASP:O	2:M:177:LYS:HG3	2.15	0.46
2:K:146:LYS:NZ	2:K:229:ASP:O	2.40	0.46
2:I:245:ASP:O	2:I:249:LYS:HG3	2.15	0.46
2:M:411:ARG:NH1	3:M:506:HOH:O	2.28	0.46
2:O:356:ASN:HB2	2:O:360:ASP:OD2	2.15	0.46
1:E:48:ALA:HB1	1:E:53:ILE:O	2.16	0.46
1:H:78:LYS:HG3	1:H:80:LEU:HB2	1.97	0.46
2:I:140:ARG:HG2	2:I:199:PRO:HG2	1.98	0.46
2:O:341:ARG:CZ	3:O:502:HOH:O	2.50	0.46
2:P:162:LYS:HE2	2:P:162:LYS:HB3	1.74	0.46
1:F:77:THR:CG2	1:F:88:VAL:HG21	2.43	0.46
2:L:393:TYR:CD1	2:L:401:PRO:HB3	2.51	0.46
2:L:373:TYR:CE1	2:M:362:MET:HG3	2.50	0.46
1:D:37:HIS:CD2	1:D:38:VAL:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:LYS:CG	1:H:80:LEU:HB3	2.41	0.45
2:I:171:TRP:N	3:I:505:HOH:O	2.27	0.45
1:F:34:LEU:HD11	2:N:257:ARG:HH12	1.80	0.45
2:O:109:PRO:CD	2:O:120:LYS:HE3	2.45	0.45
2:O:305:ASN:OD1	2:O:324:THR:HG23	2.16	0.45
2:J:312:SER:HB3	2:J:314:TYR:CE2	2.51	0.45
2:L:124:TRP:CZ3	2:L:307:LYS:HA	2.51	0.45
2:M:308:SER:O	2:M:309:ASN:HB2	2.17	0.45
2:O:393:TYR:CD1	2:O:401:PRO:HB3	2.51	0.45
1:C:39:LYS:NZ	1:C:40:ASP:OD1	2.49	0.45
1:G:73:LEU:HB3	1:G:76:PHE:CB	2.46	0.45
2:L:117:LEU:HD12	2:N:420:PRO:HG2	1.98	0.45
2:M:404:LYS:HD2	2:M:404:LYS:HA	1.80	0.45
2:K:308:SER:O	2:K:309:ASN:HB2	2.17	0.45
1:E:34:LEU:HB2	1:E:63:PHE:HE1	1.80	0.45
1:G:35:LEU:HD12	1:G:36:GLU:N	2.30	0.45
2:P:147:VAL:HG11	2:P:194:ILE:HD13	1.98	0.45
1:F:30:GLU:HA	1:F:66:VAL:O	2.15	0.45
1:H:76:PHE:C	1:H:78:LYS:N	2.67	0.45
2:M:142:HIS:HB3	2:M:144:ASP:OD1	2.17	0.45
2:M:322:GLU:HG2	2:M:422:LYS:HE3	1.98	0.45
2:M:436:ALA:O	2:M:440:MET:HG3	2.16	0.45
1:F:76:PHE:O	1:F:79:LYS:HG2	2.17	0.45
2:O:255:TYR:HB3	2:O:296:LEU:HD11	1.97	0.45
2:P:329:TYR:CD2	2:P:331:GLY:O	2.70	0.45
1:G:41:LYS:O	1:G:44:LEU:HB3	2.17	0.45
2:N:172:ASN:HA	2:N:207:GLN:HB3	1.98	0.45
1:A:33:LEU:CD2	1:A:88:VAL:HG22	2.47	0.45
2:M:330:LEU:HD22	2:M:345:LEU:HD11	1.99	0.45
2:L:373:TYR:CD1	2:M:362:MET:HG3	2.52	0.45
2:P:167:THR:N	3:P:504:HOH:O	2.23	0.45
1:G:76:PHE:HA	1:G:79:LYS:HD3	1.99	0.45
2:P:296:LEU:O	3:P:510:HOH:O	2.21	0.45
1:E:46:ASP:HA	1:E:48:ALA:N	2.32	0.44
2:K:145:VAL:HG22	2:K:394:ARG:NH1	2.31	0.44
2:O:142:HIS:HB3	2:O:144:ASP:OD1	2.17	0.44
2:O:124:TRP:CD2	2:O:307:LYS:HE2	2.52	0.44
1:D:70:LYS:HA	1:D:73:LEU:HD12	1.99	0.44
1:G:40:ASP:OD2	1:G:84:VAL:HG11	2.17	0.44
2:K:245:ASP:O	2:K:249:LYS:HG3	2.17	0.44
2:K:201:VAL:HG21	2:K:387:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:305:ASN:HD22	2:N:324:THR:CG2	2.28	0.44
2:P:305:ASN:OD1	2:P:324:THR:HG23	2.17	0.44
1:H:89:ILE:HG12	2:P:247:GLU:HG3	2.00	0.44
2:I:172:ASN:HA	2:I:207:GLN:HB3	1.99	0.44
2:K:435:GLN:OE1	2:K:435:GLN:HA	2.17	0.44
2:N:322:GLU:HG3	3:N:515:HOH:O	2.17	0.44
2:P:151:ASP:OD2	3:P:511:HOH:O	2.21	0.44
1:H:78:LYS:C	1:H:80:LEU:N	2.71	0.44
2:J:116:ILE:HD12	2:J:366:PRO:HG3	1.98	0.44
2:N:124:TRP:CZ3	2:N:307:LYS:HA	2.52	0.44
1:G:31:GLN:HB3	1:G:89:ILE:O	2.18	0.44
2:I:290:VAL:HG13	2:I:292:LEU:HG	2.00	0.44
1:C:89:ILE:HG23	2:K:247:GLU:HB3	1.97	0.44
2:N:245:ASP:O	2:N:249:LYS:HG3	2.18	0.44
2:O:393:TYR:CG	2:O:401:PRO:HB3	2.52	0.44
1:H:80:LEU:HD22	1:H:83:LYS:CB	2.47	0.44
2:J:111:TRP:CZ3	2:J:123:LEU:HD21	2.53	0.44
2:L:243:SER:O	2:L:248:GLY:HA3	2.18	0.44
1:E:43:LYS:HB3	1:E:43:LYS:HE2	1.74	0.44
1:H:83:LYS:HB2	1:H:84:VAL:H	0.93	0.44
2:J:177:LYS:HB2	2:J:178:PRO:HD2	1.99	0.44
2:J:385:THR:HG23	2:J:433:ALA:HA	2.00	0.44
2:L:255:TYR:HB3	2:L:296:LEU:HD11	1.98	0.44
2:M:397:HIS:HB3	2:M:399:ARG:NH1	2.32	0.44
2:N:411:ARG:HG3	2:N:428:TYR:CD1	2.53	0.44
2:N:422:LYS:H	2:N:422:LYS:HD3	1.83	0.44
1:F:89:ILE:HG12	1:F:90:GLU:H	1.83	0.44
1:H:44:LEU:HB2	1:H:78:LYS:HE2	1.99	0.44
2:K:293:PRO:HD2	3:K:523:HOH:O	2.18	0.44
2:O:158:HIS:HA	2:O:159:PRO:HD3	1.84	0.44
1:D:78:LYS:HA	1:D:81:ALA:CB	2.48	0.43
1:E:53:ILE:HG23	1:E:67:THR:O	2.17	0.43
1:H:32:TYR:HB2	1:H:89:ILE:HB	2.00	0.43
2:J:329:TYR:CG	2:J:330:LEU:N	2.86	0.43
2:L:140:ARG:NH2	3:L:518:HOH:O	2.50	0.43
2:M:245:ASP:O	2:M:249:LYS:HG3	2.18	0.43
2:N:438:LYS:HE3	2:N:438:LYS:HB3	1.90	0.43
2:P:309:ASN:O	2:P:417:LEU:HD13	2.17	0.43
1:A:61:ILE:HA	3:A:211:HOH:O	2.17	0.43
1:E:33:LEU:HA	1:E:87:ASP:O	2.19	0.43
2:N:212:LYS:HE3	3:N:586:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:163:ALA:HB3	3:N:564:HOH:O	2.17	0.43
1:H:71:GLN:HG3	1:H:72:LYS:HG2	1.95	0.43
2:L:109:PRO:HD3	2:L:133:TYR:CE2	2.53	0.43
1:F:32:TYR:CE1	1:F:65:LYS:HB2	2.53	0.43
1:F:89:ILE:HG12	1:F:90:GLU:N	2.32	0.43
2:J:322:GLU:HG3	3:J:527:HOH:O	2.19	0.43
2:N:436:ALA:O	2:N:440:MET:HG3	2.19	0.43
1:A:72:LYS:C	1:A:75:PRO:HD2	2.38	0.43
1:A:53:ILE:HG23	1:A:72:LYS:HE3	2.00	0.43
1:E:50:GLN:C	1:E:51:PHE:HD1	2.22	0.43
2:P:146:LYS:HB3	2:P:231:HIS:CD2	2.54	0.43
1:C:73:LEU:HA	1:C:76:PHE:HB3	2.00	0.43
1:F:41:LYS:HE3	1:F:41:LYS:HB3	1.77	0.43
1:H:84:VAL:HB	1:H:85:GLY:H	1.15	0.43
2:I:161:LEU:O	2:I:165:VAL:HG23	2.18	0.43
1:F:88:VAL:O	2:N:247:GLU:OE1	2.37	0.43
1:G:43:LYS:C	1:G:83:LYS:HE2	2.39	0.43
2:I:432:ARG:CZ	2:I:435:GLN:HG3	2.49	0.42
2:O:142:HIS:CE1	2:O:395:GLU:HG3	2.53	0.42
2:O:432:ARG:CZ	2:O:435:GLN:HG3	2.48	0.42
1:H:79:LYS:H	1:H:79:LYS:HG3	1.53	0.42
2:M:173:TYR:OH	2:M:225:ASP:OD2	2.22	0.42
2:O:318:GLY:CA	2:O:424:VAL:HG13	2.49	0.42
1:A:51:PHE:O	1:A:72:LYS:CE	2.67	0.42
1:B:31:GLN:HG3	1:B:73:LEU:HD13	2.01	0.42
2:I:104:VAL:HG22	2:I:105:ILE:HD12	2.00	0.42
2:K:411:ARG:NH1	2:K:412:LYS:HZ3	2.17	0.42
2:L:422:LYS:NZ	3:L:521:HOH:O	2.52	0.42
2:M:225:ASP:HA	3:M:517:HOH:O	2.19	0.42
1:B:52:HIS:ND1	1:B:52:HIS:O	2.51	0.42
1:B:60:GLU:HG2	2:J:261:TYR:CZ	2.55	0.42
1:A:47:THR:HG22	1:A:76:PHE:HD1	1.84	0.42
1:D:32:TYR:HB2	1:D:89:ILE:HB	2.02	0.42
1:F:50:GLN:O	1:F:51:PHE:HD1	2.03	0.42
2:O:360:ASP:HB3	2:O:365:ILE:HB	2.00	0.42
1:H:69:GLU:HG3	1:H:71:GLN:HB2	2.01	0.42
2:I:215:ASP:OD2	2:I:217:TYR:HB3	2.20	0.42
2:M:438:LYS:NZ	3:M:524:HOH:O	2.52	0.42
2:N:138:ILE:C	3:N:509:HOH:O	2.58	0.42
2:P:246:ARG:O	2:P:250:VAL:HG23	2.20	0.42
2:P:411:ARG:HD2	2:P:428:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:308:SER:O	2:O:309:ASN:HB2	2.18	0.42
2:O:317:GLN:OE1	2:O:425:ILE:HG12	2.19	0.42
2:O:411:ARG:HD2	2:O:428:TYR:CZ	2.55	0.42
1:D:46:ASP:O	1:D:50:GLN:HB3	2.20	0.42
1:F:80:LEU:HB3	1:F:84:VAL:HG23	2.02	0.42
1:G:78:LYS:O	1:G:82:GLU:OE2	2.37	0.42
2:M:171:TRP:HD1	2:M:173:TYR:CE2	2.38	0.42
2:N:394:ARG:HE	2:N:400:LYS:HB3	1.84	0.42
1:C:60:GLU:N	1:C:60:GLU:OE1	2.47	0.42
2:J:411:ARG:HD2	2:J:428:TYR:CE1	2.55	0.42
2:O:142:HIS:HB2	2:O:145:VAL:HG23	2.01	0.42
2:O:328:GLY:N	3:O:508:HOH:O	2.23	0.42
1:E:80:LEU:C	1:E:82:GLU:N	2.71	0.41
1:F:46:ASP:N	3:F:201:HOH:O	2.05	0.41
1:G:49:GLU:H	1:G:49:GLU:CD	2.23	0.41
2:I:348:THR:O	2:I:369:TYR:HA	2.19	0.41
2:K:169:GLY:HA3	3:K:642:HOH:O	2.20	0.41
2:L:394:ARG:HA	2:L:399:ARG:O	2.20	0.41
2:M:212:LYS:HE3	2:M:212:LYS:HB2	1.84	0.41
2:M:281:ASP:OD1	2:M:319:ARG:NH1	2.53	0.41
2:N:158:HIS:HA	2:N:159:PRO:HD2	1.88	0.41
1:A:72:LYS:HA	1:A:75:PRO:HD2	2.01	0.41
2:M:284:ARG:NE	3:M:525:HOH:O	2.53	0.41
2:L:362:MET:HE1	2:M:345:LEU:HD21	2.02	0.41
2:P:371:LEU:HD12	2:P:371:LEU:HA	1.85	0.41
1:H:39:LYS:HG2	1:H:39:LYS:O	2.20	0.41
2:I:185:GLY:O	2:I:189:GLN:HG3	2.21	0.41
2:K:390:ILE:O	2:K:394:ARG:HG3	2.20	0.41
2:P:323:PHE:HB3	2:P:431:VAL:HG23	2.02	0.41
2:O:397:HIS:CD2	2:O:397:HIS:N	2.87	0.41
1:C:51:PHE:O	1:C:72:LYS:HB3	2.21	0.41
1:F:47:THR:HG21	1:F:79:LYS:HB2	2.02	0.41
1:G:35:LEU:CD2	1:G:38:VAL:HA	2.51	0.41
2:L:396:ARG:HD3	2:L:397:HIS:CE1	2.55	0.41
1:H:77:THR:O	1:H:78:LYS:CB	2.67	0.41
2:I:109:PRO:HD2	2:I:120:LYS:HE2	2.03	0.41
2:L:404:LYS:HE2	2:L:404:LYS:HB3	1.79	0.41
2:N:125:PHE:CG	2:N:126:ALA:N	2.89	0.41
2:P:263:ALA:CB	2:P:298:HIS:CD2	3.04	0.41
2:I:243:SER:O	2:I:248:GLY:HA3	2.21	0.41
2:K:312:SER:HB3	2:K:314:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:324:THR:HG22	2:L:430:GLU:HA	2.01	0.41
2:M:224:VAL:HG13	2:M:261:TYR:CE2	2.55	0.41
2:L:359:LEU:HD13	2:M:330:LEU:HD21	2.02	0.41
2:N:322:GLU:OE1	2:N:407:HIS:NE2	2.31	0.41
2:P:228:ASN:OD1	2:P:261:TYR:OH	2.23	0.41
2:P:272:SER:HB3	2:P:376:SER:HA	2.03	0.41
1:H:35:LEU:HD11	1:H:44:LEU:CD2	2.34	0.41
2:J:357:THR:O	2:J:361:GLN:HG2	2.21	0.41
2:N:122:TYR:CD1	2:N:371:LEU:HD11	2.56	0.41
2:O:324:THR:HG22	2:O:430:GLU:HA	2.03	0.41
1:A:41:LYS:O	1:A:44:LEU:HB3	2.21	0.41
1:D:62:GLY:HA2	3:D:203:HOH:O	2.20	0.41
1:D:78:LYS:HE2	1:D:78:LYS:HB3	1.88	0.41
2:K:338:GLY:HA3	3:K:556:HOH:O	2.21	0.41
1:G:80:LEU:HA	1:G:80:LEU:HD23	1.57	0.41
2:M:206:TYR:OH	2:M:226:ALA:HA	2.20	0.41
2:N:146:LYS:HB3	2:N:231:HIS:CD2	2.56	0.41
2:O:352:LYS:HB3	3:O:541:HOH:O	2.20	0.41
2:O:396:ARG:HB3	2:O:397:HIS:HD2	1.86	0.41
1:A:33:LEU:HD23	1:A:88:VAL:HG22	2.03	0.41
1:D:47:THR:HG22	1:D:76:PHE:CE1	2.56	0.41
1:G:38:VAL:O	1:G:40:ASP:N	2.54	0.41
1:H:35:LEU:C	1:H:36:GLU:HG3	2.41	0.41
2:I:308:SER:O	2:I:309:ASN:HB2	2.21	0.41
2:J:356:ASN:HB2	2:J:360:ASP:OD2	2.21	0.41
2:L:290:VAL:HG13	2:L:292:LEU:HG	2.02	0.41
2:M:281:ASP:HA	3:M:526:HOH:O	2.20	0.41
2:M:305:ASN:OD1	2:M:324:THR:HG23	2.21	0.41
2:N:348:THR:O	2:N:369:TYR:HA	2.20	0.41
2:P:246:ARG:CG	2:P:247:GLU:HB2	2.50	0.41
1:E:73:LEU:O	1:E:77:THR:HG23	2.21	0.40
2:I:245:ASP:CG	3:I:502:HOH:O	2.58	0.40
2:I:305:ASN:OD1	2:I:324:THR:HG23	2.21	0.40
2:N:393:TYR:HD2	2:N:401:PRO:HD3	1.86	0.40
2:N:419:LYS:O	3:N:502:HOH:O	2.22	0.40
2:O:397:HIS:HB3	2:O:399:ARG:HE	1.86	0.40
1:D:81:ALA:HA	1:D:84:VAL:O	2.22	0.40
1:F:80:LEU:O	1:F:83:LYS:N	2.52	0.40
2:K:161:LEU:O	2:K:165:VAL:HG23	2.22	0.40
2:M:324:THR:HG22	2:M:430:GLU:HA	2.03	0.40
2:P:394:ARG:NE	2:P:400:LYS:HG2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:206:TYR:OH	2:L:226:ALA:HA	2.22	0.40
2:N:411:ARG:HG3	2:N:428:TYR:CG	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:620:HOH:O	3:O:535:HOH:O[1_455]	2.02	0.18
2:M:434:TYR:OH	2:O:336:GLN:O[1_456]	2.09	0.11

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	59/100 (59%)	59 (100%)	0	0	100	100
1	B	58/100 (58%)	56 (97%)	2 (3%)	0	100	100
1	C	58/100 (58%)	54 (93%)	2 (3%)	2 (3%)	3	2
1	D	58/100 (58%)	54 (93%)	4 (7%)	0	100	100
1	E	59/100 (59%)	53 (90%)	4 (7%)	2 (3%)	3	2
1	F	60/100 (60%)	51 (85%)	6 (10%)	3 (5%)	2	0
1	G	60/100 (60%)	53 (88%)	3 (5%)	4 (7%)	1	0
1	H	60/100 (60%)	44 (73%)	7 (12%)	9 (15%)	0	0
2	I	335/343 (98%)	327 (98%)	8 (2%)	0	100	100
2	J	335/343 (98%)	329 (98%)	6 (2%)	0	100	100
2	K	333/343 (97%)	327 (98%)	5 (2%)	1 (0%)	41	47
2	L	335/343 (98%)	324 (97%)	9 (3%)	2 (1%)	25	27
2	M	329/343 (96%)	321 (98%)	6 (2%)	2 (1%)	25	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	333/343 (97%)	327 (98%)	6 (2%)	0	100	100
2	O	333/343 (97%)	322 (97%)	9 (3%)	2 (1%)	25	27
2	P	335/343 (98%)	326 (97%)	7 (2%)	2 (1%)	25	27
All	All	3140/3544 (89%)	3027 (96%)	84 (3%)	29 (1%)	17	17

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	72	LYS
2	L	398	HIS
1	E	42	SER
1	E	82	GLU
2	M	106	SER
1	F	79	LYS
1	G	39	LYS
2	O	337	ASP
1	H	42	SER
1	H	46	ASP
1	H	47	THR
1	H	71	GLN
1	H	83	LYS
2	P	332	GLU
1	G	73	LEU
1	H	41	LYS
1	H	52	HIS
2	L	177	LYS
1	G	48	ALA
1	C	70	LYS
1	H	78	LYS
2	K	177	LYS
1	F	77	THR
1	G	81	ALA
2	P	177	LYS
1	H	84	VAL
1	F	68	GLY
2	M	177	LYS
2	O	331	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	52/82 (63%)	52 (100%)	0	100	100
1	B	51/82 (62%)	51 (100%)	0	100	100
1	C	51/82 (62%)	51 (100%)	0	100	100
1	D	50/82 (61%)	49 (98%)	1 (2%)	55	66
1	E	50/82 (61%)	48 (96%)	2 (4%)	31	39
1	F	51/82 (62%)	51 (100%)	0	100	100
1	G	50/82 (61%)	44 (88%)	6 (12%)	5	4
1	H	51/82 (62%)	42 (82%)	9 (18%)	2	1
2	I	277/283 (98%)	275 (99%)	2 (1%)	84	91
2	J	277/283 (98%)	274 (99%)	3 (1%)	73	84
2	K	275/283 (97%)	271 (98%)	4 (2%)	65	76
2	L	277/283 (98%)	274 (99%)	3 (1%)	73	84
2	M	274/283 (97%)	268 (98%)	6 (2%)	52	63
2	N	275/283 (97%)	269 (98%)	6 (2%)	52	63
2	O	275/283 (97%)	273 (99%)	2 (1%)	84	91
2	P	277/283 (98%)	272 (98%)	5 (2%)	59	70
All	All	2613/2920 (90%)	2564 (98%)	49 (2%)	57	68

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	255	TYR
2	I	324	THR
2	J	255	TYR
2	J	285	LYS
2	J	375	THR
2	K	255	TYR
2	K	342	VAL
2	K	375	THR

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Mol	Chain	Res	Type
2	K	412	LYS
1	D	78	LYS
2	L	104	VAL
2	L	255	TYR
2	L	435	GLN
1	E	41	LYS
1	E	78	LYS
2	M	117	LEU
2	M	118	GLU
2	M	168	ASN
2	M	250	VAL
2	M	255	TYR
2	M	332	GLU
2	N	137	GLN
2	N	255	TYR
2	N	297	LYS
2	N	400	LYS
2	N	404	LYS
2	N	419	LYS
1	G	41	LYS
1	G	47	THR
1	G	49	GLU
1	G	59	GLU
1	G	78	LYS
1	G	82	GLU
2	O	255	TYR
2	O	257	ARG
1	H	38	VAL
1	H	39	LYS
1	H	40	ASP
1	H	53	ILE
1	H	71	GLN
1	H	72	LYS
1	H	76	PHE
1	H	79	LYS
1	H	80	LEU
2	P	106	SER
2	P	151	ASP
2	P	232	GLU
2	P	255	TYR
2	P	298	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
2	I	137	GLN
1	D	37	HIS
1	E	50	GLN
2	N	142	HIS
2	N	305	ASN
2	N	397	HIS
2	O	336	GLN
2	O	408	HIS

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

There are no ligands in this entry.

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, 95^{th} 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	61/100 (61%)	0.89	8 (13%) 3 5	39, 59, 79, 88	0
1	B	60/100 (60%)	1.05	12 (20%) 1 2	43, 60, 82, 88	0
1	C	60/100 (60%)	1.01	11 (18%) 1 2	44, 60, 79, 90	0
1	D	60/100 (60%)	2.24	29 (48%) 0 0	50, 80, 107, 116	0
1	E	61/100 (61%)	2.85	43 (70%) 0 0	57, 95, 110, 122	0
1	F	62/100 (62%)	2.57	38 (61%) 0 0	57, 92, 110, 115	0
1	G	62/100 (62%)	3.12	46 (74%) 0 0	61, 95, 121, 124	0
1	H	62/100 (62%)	4.22	48 (77%) 0 0	68, 110, 136, 144	0
2	I	337/343 (98%)	0.09	2 (0%) 89 93	26, 37, 53, 77	0
2	J	337/343 (98%)	0.02	2 (0%) 89 93	27, 38, 56, 74	0
2	K	335/343 (97%)	0.15	5 (1%) 73 81	28, 38, 52, 80	0
2	L	337/343 (98%)	0.39	10 (2%) 50 61	33, 45, 63, 119	0
2	M	333/343 (97%)	0.36	15 (4%) 33 46	29, 44, 71, 95	0
2	N	335/343 (97%)	0.45	17 (5%) 28 40	29, 46, 75, 95	0
2	O	335/343 (97%)	0.32	12 (3%) 42 55	31, 47, 72, 103	0
2	P	337/343 (98%)	0.56	26 (7%) 13 20	34, 54, 78, 115	0
All	All	3174/3544 (89%)	0.59	324 (10%) 6 11	26, 46, 95, 144	0

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	104	VAL	16.8
2	P	104	VAL	16.5
2	L	105	ILE	16.3
1	H	84	VAL	14.6
1	H	75	PRO	14.4

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Mol	Chain	Res	Type	RSRZ
2	M	105	ILE	13.2
1	G	84	VAL	11.3
2	P	106	SER	10.7
1	H	72	LYS	9.7
1	G	83	LYS	9.6
1	H	85	GLY	9.6
1	H	77	THR	9.5
1	H	53	ILE	9.3
2	P	105	ILE	9.2
1	E	53	ILE	8.9
2	M	104	VAL	8.8
1	D	68	GLY	8.5
1	H	51	PHE	8.3
1	F	68	GLY	8.0
1	F	53	ILE	7.8
1	H	68	GLY	7.7
1	H	76	PHE	7.3
1	H	83	LYS	7.3
1	H	71	GLN	7.3
1	E	68	GLY	6.7
1	H	54	HIS	6.7
1	H	86	ALA	6.7
1	E	45	LEU	6.7
1	G	53	ILE	6.6
1	E	52	HIS	6.4
1	F	83	LYS	6.2
1	H	49	GLU	6.1
1	H	33	LEU	6.1
1	D	84	VAL	6.0
2	M	106	SER	6.0
2	K	106	SER	5.9
1	E	54	HIS	5.9
1	H	47	THR	5.8
1	H	44	LEU	5.8
1	F	80	LEU	5.6
1	H	45	LEU	5.4
2	P	246	ARG	5.4
1	D	53	ILE	5.3
1	E	67	THR	5.3
1	H	38	VAL	5.3
1	H	89	ILE	5.3
1	E	44	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	G	70	LYS	5.2
1	G	85	GLY	5.2
2	L	106	SER	5.1
1	F	76	PHE	5.1
1	H	50	GLN	5.1
2	P	251	LEU	5.0
1	F	69	GLU	5.0
1	H	81	ALA	5.0
1	D	82	GLU	4.8
1	E	49	GLU	4.8
1	E	76	PHE	4.8
1	H	35	LEU	4.8
1	G	72	LYS	4.7
1	H	74	ALA	4.7
1	G	78	LYS	4.7
1	H	52	HIS	4.7
1	H	80	LEU	4.7
1	D	81	ALA	4.7
1	F	45	LEU	4.7
1	G	66	VAL	4.6
1	H	88	VAL	4.6
1	G	86	ALA	4.6
1	F	52	HIS	4.6
1	E	84	VAL	4.5
1	F	46	ASP	4.5
1	A	72	LYS	4.5
1	G	49	GLU	4.5
1	D	52	HIS	4.5
1	C	68	GLY	4.5
1	E	83	LYS	4.5
1	D	46	ASP	4.5
1	E	70	LYS	4.4
1	H	34	LEU	4.4
1	G	68	GLY	4.4
1	F	90	GLU	4.4
1	D	49	GLU	4.4
1	G	88	VAL	4.4
1	F	50	GLN	4.3
1	E	89	ILE	4.3
1	G	77	THR	4.3
1	E	86	ALA	4.3
1	H	67	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	78	LYS	4.2
2	N	286	THR	4.2
1	G	81	ALA	4.2
1	B	84	VAL	4.1
1	E	85	GLY	4.1
1	G	50	GLN	4.1
1	F	44	LEU	4.1
1	C	70	LYS	4.1
2	M	212	LYS	4.1
1	G	67	THR	4.1
2	P	419	LYS	4.1
1	H	73	LEU	4.1
1	F	75	PRO	4.0
2	O	336	GLN	4.0
1	G	69	GLU	4.0
1	G	44	LEU	3.9
1	G	54	HIS	3.9
1	G	52	HIS	3.9
2	P	250	VAL	3.9
1	F	81	ALA	3.9
1	B	72	LYS	3.9
1	D	71	GLN	3.8
1	F	84	VAL	3.8
1	F	88	VAL	3.8
1	D	50	GLN	3.8
1	G	82	GLU	3.8
2	P	178	PRO	3.8
1	B	83	LYS	3.8
1	G	51	PHE	3.7
1	D	55	ALA	3.7
1	G	38	VAL	3.7
1	H	78	LYS	3.7
1	D	76	PHE	3.7
1	D	69	GLU	3.7
1	H	70	LYS	3.6
1	G	32	TYR	3.6
1	E	78	LYS	3.6
1	G	55	ALA	3.6
1	E	30	GLU	3.6
1	D	73	LEU	3.6
2	N	106	SER	3.6
1	F	31	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
2	N	247	GLU	3.5
2	P	176	GLY	3.5
1	B	71	GLN	3.5
1	E	77	THR	3.5
1	H	69	GLU	3.5
1	D	70	LYS	3.5
1	G	79	LYS	3.4
1	E	55	ALA	3.4
1	H	32	TYR	3.4
1	E	63	PHE	3.4
1	D	54	HIS	3.4
1	F	48	ALA	3.3
1	G	76	PHE	3.3
2	L	398	HIS	3.3
1	D	80	LEU	3.3
1	E	81	ALA	3.3
1	F	72	LYS	3.3
2	I	104	VAL	3.2
1	G	36	GLU	3.2
1	G	80	LEU	3.2
2	N	439	MET	3.2
2	N	396	ARG	3.2
1	D	79	LYS	3.2
1	F	73	LEU	3.2
1	F	78	LYS	3.2
1	F	85	GLY	3.1
1	C	54	HIS	3.1
1	D	67	THR	3.1
2	O	438	LYS	3.1
1	F	33	LEU	3.1
2	N	398	HIS	3.1
1	B	53	ILE	3.1
1	A	71	GLN	3.1
1	E	43	LYS	3.0
1	D	83	LYS	3.0
1	H	82	GLU	3.0
1	G	39	LYS	3.0
2	O	212	LYS	3.0
2	M	178	PRO	3.0
1	E	82	GLU	3.0
2	N	255	TYR	3.0
2	P	298	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	365	ILE	3.0
1	C	72	LYS	3.0
1	E	42	SER	2.9
1	F	43	LYS	2.9
2	K	285	LYS	2.9
2	O	412	LYS	2.9
1	A	84	VAL	2.9
1	D	51	PHE	2.9
1	H	66	VAL	2.9
2	N	244	LEU	2.9
2	P	257	ARG	2.9
2	O	250	VAL	2.9
1	E	72	LYS	2.9
1	D	48	ALA	2.9
1	E	88	VAL	2.9
2	M	332	GLU	2.9
1	E	38	VAL	2.9
1	G	33	LEU	2.9
1	G	34	LEU	2.9
1	B	42	SER	2.8
2	N	285	LYS	2.8
1	F	51	PHE	2.8
1	E	62	GLY	2.8
1	B	79	LYS	2.8
1	D	77	THR	2.8
1	B	69	GLU	2.8
1	G	35	LEU	2.8
2	O	335	ASP	2.8
2	P	212	LYS	2.8
2	M	181	GLY	2.8
2	N	246	ARG	2.8
1	F	49	GLU	2.8
2	P	175	ASP	2.8
2	P	177	LYS	2.8
1	E	59	GLU	2.8
1	F	70	LYS	2.8
2	O	439	MET	2.7
1	G	75	PRO	2.7
1	H	36	GLU	2.7
1	C	81	ALA	2.7
1	E	34	LEU	2.7
1	H	55	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	M	169	GLY	2.7
2	M	171	TRP	2.6
1	C	67	THR	2.6
1	D	33	LEU	2.6
1	F	79	LYS	2.6
1	F	55	ALA	2.6
2	L	236	ILE	2.6
1	E	33	LEU	2.6
1	G	43	LYS	2.6
2	N	393	TYR	2.6
1	F	71	GLN	2.6
1	E	61	ILE	2.6
1	B	35	LEU	2.6
1	E	66	VAL	2.6
1	E	69	GLU	2.6
1	F	82	GLU	2.6
2	P	145	VAL	2.6
1	D	31	GLN	2.6
1	A	83	LYS	2.6
1	F	32	TYR	2.5
1	A	68	GLY	2.5
2	J	211	GLU	2.5
2	M	168	ASN	2.5
1	D	74	ALA	2.5
1	E	75	PRO	2.5
1	H	46	ASP	2.5
1	B	52	HIS	2.5
2	P	284	ARG	2.5
1	G	48	ALA	2.5
1	G	74	ALA	2.5
2	M	334	TYR	2.5
2	I	211	GLU	2.5
1	B	38	VAL	2.5
1	D	37	HIS	2.5
1	F	30	GLU	2.5
1	G	63	PHE	2.5
2	P	244	LEU	2.5
2	O	176	GLY	2.4
1	F	87	ASP	2.4
1	C	66	VAL	2.4
1	F	86	ALA	2.4
1	F	89	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	42	SER	2.4
2	N	404	LYS	2.4
2	K	396	ARG	2.4
1	H	39	LYS	2.4
1	E	73	LEU	2.4
1	C	69	GLU	2.4
1	H	48	ALA	2.4
1	G	46	ASP	2.4
1	E	46	ASP	2.4
2	L	176	GLY	2.4
1	A	69	GLU	2.4
2	P	319	ARG	2.3
2	K	255	TYR	2.3
1	C	85	GLY	2.3
2	K	394	ARG	2.3
2	P	167	THR	2.3
1	D	88	VAL	2.3
1	G	71	GLN	2.3
2	M	117	LEU	2.3
2	J	104	VAL	2.3
1	G	30	GLU	2.3
1	H	30	GLU	2.3
2	L	132	SER	2.3
2	L	272	SER	2.3
1	H	37	HIS	2.3
2	P	180	SER	2.3
1	G	91	LYS	2.3
1	E	51	PHE	2.2
2	O	106	SER	2.2
1	F	66	VAL	2.2
1	E	48	ALA	2.2
2	N	403	ALA	2.2
1	E	32	TYR	2.2
1	G	37	HIS	2.2
1	H	63	PHE	2.2
2	N	287	GLU	2.2
2	P	211	GLU	2.2
2	P	179	VAL	2.2
2	P	417	LEU	2.2
1	B	82	GLU	2.2
2	N	399	ARG	2.1
2	P	299	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	79	LYS	2.1
1	A	53	ILE	2.1
1	H	31	GLN	2.1
2	P	425	ILE	2.1
2	L	244	LEU	2.1
1	G	62	GLY	2.1
1	C	55	ALA	2.1
1	E	74	ALA	2.1
2	P	201	VAL	2.1
2	O	213	GLY	2.1
1	F	74	ALA	2.1
1	G	47	THR	2.1
2	N	319	ARG	2.1
1	H	87	ASP	2.1
2	O	333	THR	2.1
2	N	288	ASN	2.1
2	M	217	TYR	2.1
2	M	267	VAL	2.1
1	G	40	ASP	2.0
1	E	50	GLN	2.0
2	O	334	TYR	2.0
2	M	213	GLY	2.0
1	C	76	PHE	2.0
1	A	73	LEU	2.0
1	E	71	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.