Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2023 – 05:15 pm GMT

PDB ID	:	1VYJ
Title	:	Structural and biochemical studies of human PCNA complexes provide the basis for association with CDK/cyclin and rationale for inhibitor design
Authors	:	Kontopidis, G.; Wu, S.; Zheleva, D.; Taylor, P.; Mcinnes, C.; Lane, D.; Fischer, P.; Walkinshaw, M.D.
Deposited on	:	2004-04-30
Resolution	:	2.80 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:

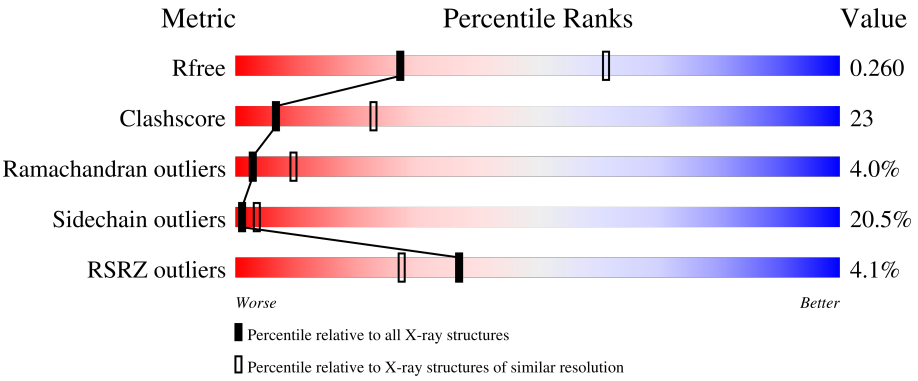
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	261	3% 56% 33% 7%
1	C	261	2% 58% 29% 9%
1	E	261	4% 57% 31% 9%
1	G	261	4% 51% 35% 13%
1	I	261	3% 52% 37% 7%

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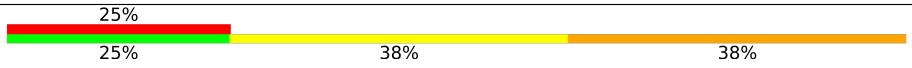
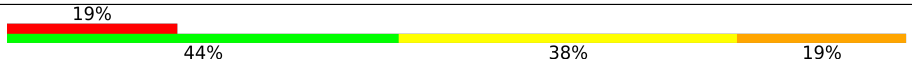
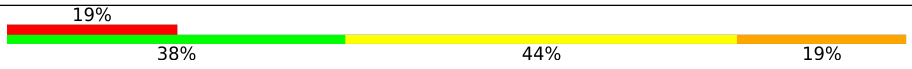
Mol	Chain	Length	Quality of chain
1	K	261	
2	B	16	
2	D	16	
2	F	16	
2	H	16	
2	J	16	
2	L	16	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13057 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 PROLIFERATING CELL NUCLEAR ANTIGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1980	1242	324	398	16			
1	C	257	Total	C	N	O	S	0	3	0
			2005	1257	328	404	16			
1	E	257	Total	C	N	O	S	0	0	0
			1980	1242	324	398	16			
1	G	260	Total	C	N	O	S	0	0	0
			2002	1254	327	405	16			
1	I	257	Total	C	N	O	S	0	0	0
			1980	1242	324	398	16			
1	K	257	Total	C	N	O	S	0	0	0
			1980	1242	324	398	16			

- Molecule 2 is a protein called SMALL PEPTIDE SAVLQKKITDYFHPKK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	0	0	0
			135	89	23	23			
2	D	16	Total	C	N	O	0	0	0
			135	89	23	23			
2	F	16	Total	C	N	O	0	0	0
			135	89	23	23			
2	H	16	Total	C	N	O	0	0	0
			135	89	23	23			
2	J	16	Total	C	N	O	0	0	0
			135	89	23	23			
2	L	16	Total	C	N	O	0	0	0
			135	89	23	23			

- Molecule 3 is water.

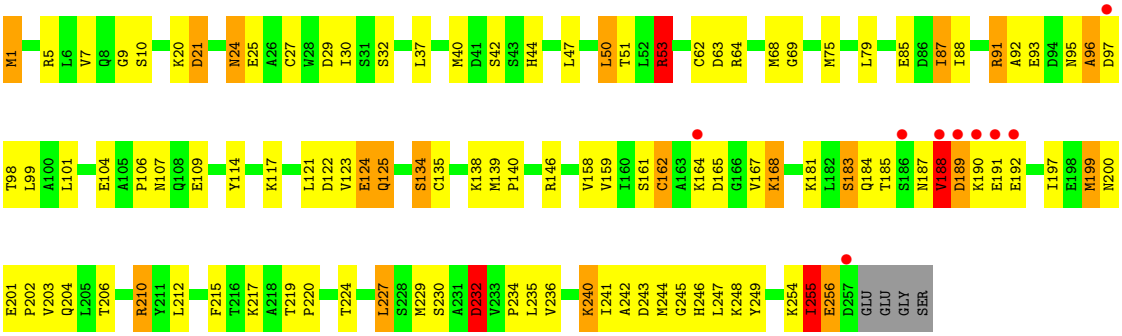
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total O 41 41	0	0
3	B	3	Total O 3 3	0	0
3	C	50	Total O 50 50	0	0
3	D	3	Total O 3 3	0	0
3	E	59	Total O 59 59	0	0
3	G	51	Total O 51 51	0	0
3	H	5	Total O 5 5	0	0
3	I	56	Total O 56 56	0	0
3	J	5	Total O 5 5	0	0
3	K	45	Total O 45 45	0	0
3	L	2	Total O 2 2	0	0

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.

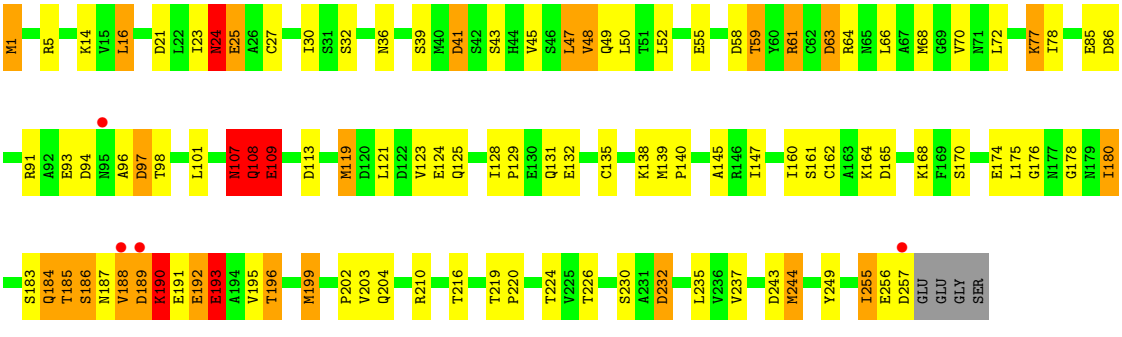
• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

Chain A:



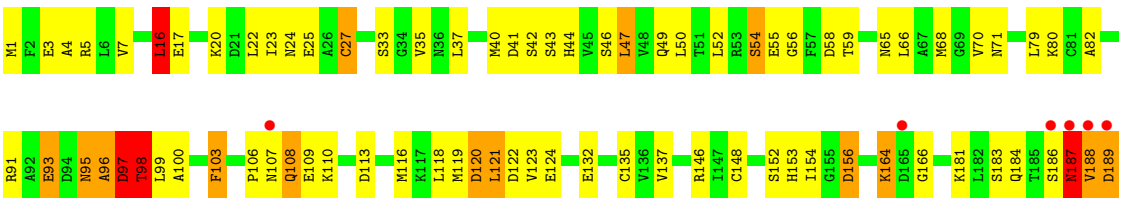
• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

Chain C:



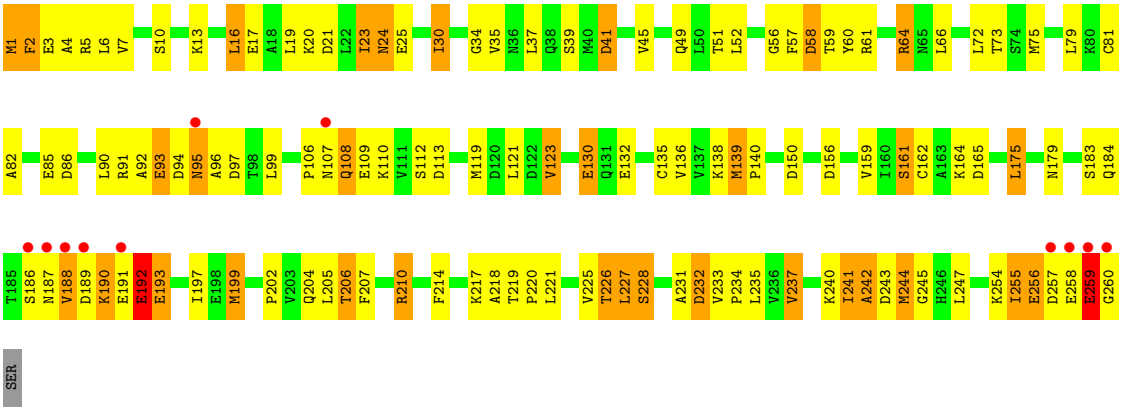
• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

Chain E:



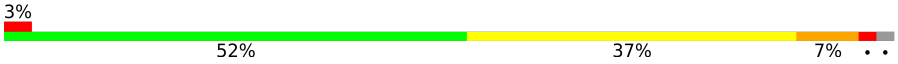
• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

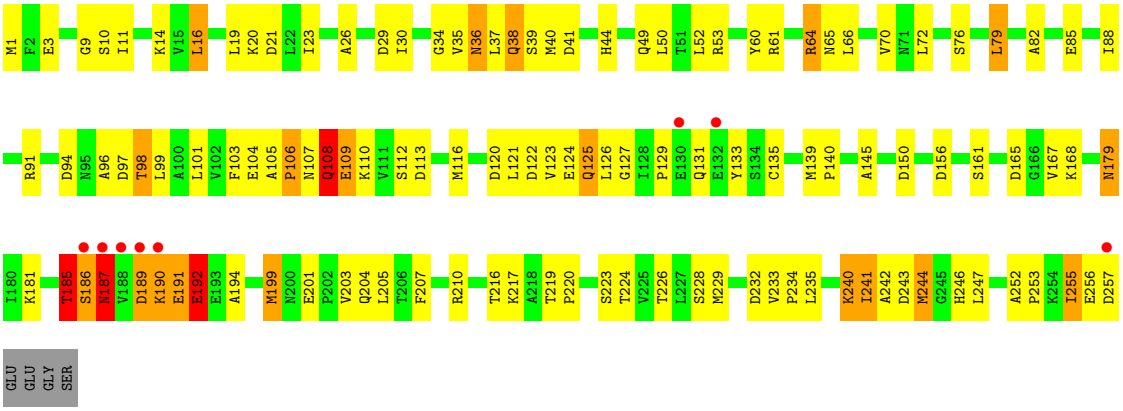
Chain G:



• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

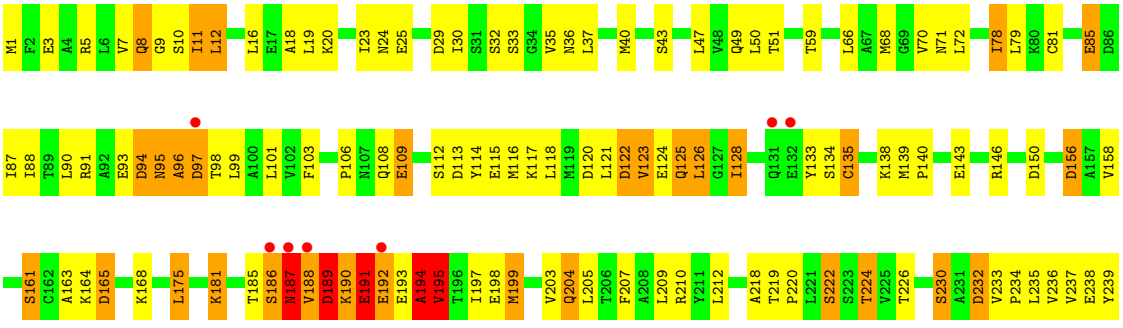
Chain I:

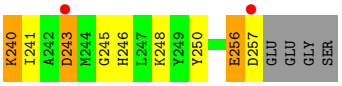




• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

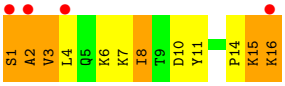
Chain K:





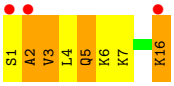
• Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK

Chain B:



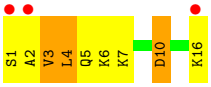
• Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK

Chain D:



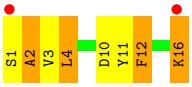
• Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK

Chain F:



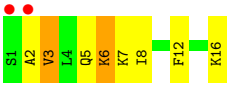
• Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK

Chain H:



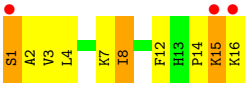
• Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK

Chain J:



• Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.10Å 119.10Å 305.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.00 – 2.80 13.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (14.00-2.80) 99.5 (13.99-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.256 0.191 , 0.260	Depositor DCC
R_{free} test set	1917 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13057	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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	0.63	1/2006 (0.0%)	1.11	11/2710 (0.4%)
1	C	0.84	1/2031 (0.0%)	1.15	11/2744 (0.4%)
1	E	0.66	1/2006 (0.0%)	1.11	9/2710 (0.3%)
1	G	0.65	1/2028 (0.0%)	1.12	7/2739 (0.3%)
1	I	0.67	1/2006 (0.0%)	1.13	12/2710 (0.4%)
1	K	0.65	0/2006	1.09	8/2710 (0.3%)
2	B	0.71	0/138	1.12	1/182 (0.5%)
2	D	0.55	0/138	0.87	0/182
2	F	0.66	0/138	1.14	1/182 (0.5%)
2	H	0.53	0/138	1.06	1/182 (0.5%)
2	J	0.56	0/138	0.95	0/182
2	L	0.69	0/138	1.04	0/182
All	All	0.68	5/12911 (0.0%)	1.11	61/17415 (0.4%)

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	C	0	3
1	E	0	4
1	G	0	1
1	I	0	2
1	K	0	4
All	All	0	14

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	255	ILE	C-N	20.87	1.82	1.34
1	G	255	ILE	C-N	6.81	1.49	1.34
1	A	255	ILE	C-N	5.59	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	252	ALA	C-N	-5.28	1.24	1.34
1	E	253	PRO	C-N	5.15	1.45	1.34

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	180	ILE	O-C-N	-11.38	104.50	122.70
1	I	192	GLU	O-C-N	10.51	139.51	122.70
1	A	245	GLY	O-C-N	-8.53	109.06	122.70
1	E	16	LEU	CA-CB-CG	-8.46	95.85	115.30
1	I	192	GLU	CA-C-N	-8.36	98.82	117.20
1	E	97	ASP	O-C-N	8.30	135.98	122.70
1	C	232	ASP	CB-CG-OD2	8.14	125.63	118.30
1	K	150	ASP	CB-CG-OD2	8.04	125.54	118.30
1	G	232	ASP	CB-CG-OD2	7.97	125.47	118.30
1	K	97	ASP	CB-CG-OD2	7.65	125.19	118.30
1	I	53	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	I	29	ASP	CB-CG-OD2	7.52	125.07	118.30
1	K	126	LEU	C-N-CA	-7.38	106.81	122.30
1	G	21	ASP	CB-CG-OD2	7.22	124.80	118.30
1	A	21	ASP	CB-CG-OD2	7.12	124.71	118.30
2	B	10	ASP	CB-CG-OD2	7.00	124.60	118.30
1	K	243	ASP	CB-CG-OD2	7.00	124.60	118.30
1	E	97	ASP	CA-C-N	-6.93	101.95	117.20
1	E	156	ASP	O-C-N	-6.84	111.76	122.70
1	I	16	LEU	CA-CB-CG	-6.79	99.69	115.30
1	A	53	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	K	156	ASP	CB-CG-OD2	6.70	124.33	118.30
1	I	122	ASP	CB-CG-OD2	6.60	124.24	118.30
1	E	232	ASP	CB-CG-OD2	6.59	124.23	118.30
1	I	21	ASP	CB-CG-OD2	6.58	124.22	118.30
2	F	10	ASP	CB-CG-OD2	6.49	124.14	118.30
1	C	91	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	E	122	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	232	ASP	CB-CG-OD2	6.21	123.89	118.30
1	I	165	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	165	ASP	CB-CG-OD2	6.18	123.86	118.30
1	I	94	ASP	CB-CG-OD2	6.11	123.80	118.30
1	G	86	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	69	GLY	N-CA-C	-6.01	98.08	113.10
2	H	10	ASP	CB-CG-OD2	5.96	123.67	118.30
1	C	16	LEU	CA-CB-CG	-5.79	102.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	120	ASP	CB-CG-OD2	5.78	123.50	118.30
1	G	41	ASP	CB-CG-OD2	5.77	123.50	118.30
1	K	29	ASP	CB-CG-OD2	5.77	123.49	118.30
1	E	103	PHE	C-N-CA	-5.75	107.33	121.70
1	C	77	LYS	CD-CE-NZ	5.73	124.87	111.70
1	I	41	ASP	CB-CG-OD2	5.66	123.40	118.30
1	C	193	GLU	O-C-N	-5.66	113.65	122.70
1	G	139	MET	CG-SD-CE	-5.51	91.39	100.20
1	G	165	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	41	ASP	CB-CG-OD2	5.40	123.16	118.30
1	G	58	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	63	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	117	LYS	O-C-N	-5.29	114.23	122.70
1	K	113	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	245	GLY	CA-C-N	5.25	128.74	117.20
1	A	29	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	86	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	75	MET	CG-SD-CE	-5.18	91.92	100.20
1	I	156	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	243	ASP	CB-CG-OD2	5.17	122.95	118.30
1	K	232	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	21	ASP	CB-CG-OD2	5.12	122.91	118.30
1	I	210	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	C	160	ILE	N-CA-C	-5.05	97.37	111.00
1	A	50	LEU	CB-CG-CD1	-5.02	102.47	111.00

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	107	ASN	Peptide
1	C	180	ILE	Mainchain
1	C	193	GLU	Mainchain
1	E	110	LYS	Mainchain
1	E	156	ASP	Mainchain,Peptide
1	E	98	THR	Mainchain
1	G	2	PHE	Sidechain
1	I	185	THR	Peptide
1	I	192	GLU	Peptide
1	K	133	TYR	Sidechain
1	K	194	ALA	Peptide
1	K	195	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	K	241	ILE	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	1980	0	1983	90	0
1	C	2005	0	2001	71	2
1	E	1980	0	1981	91	1
1	G	2002	0	1996	106	3
1	I	1980	0	1981	88	0
1	K	1980	0	1981	120	0
2	B	135	0	146	22	0
2	D	135	0	146	10	0
2	F	135	0	146	10	0
2	H	135	0	146	10	0
2	J	135	0	146	3	0
2	L	135	0	146	8	0
3	A	41	0	0	9	0
3	B	3	0	0	0	0
3	C	50	0	0	5	0
3	D	3	0	0	0	0
3	E	59	0	0	5	0
3	G	51	0	0	3	0
3	H	5	0	0	0	0
3	I	56	0	0	2	0
3	J	5	0	0	0	0
3	K	45	0	0	5	0
3	L	2	0	0	0	0
All	All	13057	0	12799	599	3

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 23.

All (599) 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:C:255:ILE:C	1:C:256:GLU:N	1.82	1.33
1:G:108:GLN:O	1:G:109:GLU:CG	1.82	1.24
1:E:189:ASP:OD1	1:E:189:ASP:O	1.55	1.22
2:F:2:ALA:O	2:F:3:VAL:HG13	1.08	1.20
1:G:108:GLN:O	1:G:109:GLU:HG2	1.01	1.16
2:F:2:ALA:O	2:F:3:VAL:CG1	1.92	1.16
1:C:107:ASN:ND2	1:C:108:GLN:O	1.82	1.12
1:I:110:LYS:O	1:I:110:LYS:HG3	1.43	1.12
1:C:5:ARG:HD2	3:C:2001:HOH:O	1.50	1.09
1:E:188:VAL:O	1:E:189:ASP:CG	1.90	1.08
1:I:191:GLU:O	1:I:192:GLU:HB3	1.48	1.06
1:E:5:ARG:HB3	1:E:59:THR:HB	1.42	1.01
2:D:2:ALA:O	2:D:3:VAL:HG23	1.60	1.01
1:I:109:GLU:HA	1:I:109:GLU:OE1	1.61	0.97
1:A:40:MET:SD	2:B:8:ILE:CG2	2.52	0.96
1:K:187:ASN:HD22	1:K:188:VAL:N	1.62	0.96
1:I:192:GLU:O	1:I:192:GLU:HG2	1.59	0.96
1:C:107:ASN:HD21	1:C:109:GLU:HB2	1.31	0.96
1:I:241:ILE:HG12	1:I:241:ILE:O	1.63	0.96
1:I:109:GLU:OE1	1:I:109:GLU:CA	2.15	0.95
1:G:175:LEU:HD23	1:G:175:LEU:H	1.32	0.94
1:G:193:GLU:O	1:G:193:GLU:HG2	1.68	0.93
1:C:184:GLN:O	1:C:185:THR:O	1.86	0.92
1:K:256:GLU:O	1:K:257:ASP:HB2	1.68	0.91
1:A:188:VAL:O	1:A:189:ASP:HB2	1.67	0.91
1:E:95:ASN:O	1:E:96:ALA:O	1.89	0.91
1:C:107:ASN:ND2	1:C:109:GLU:HB2	1.84	0.91
2:D:1:SER:O	2:D:2:ALA:HB3	1.71	0.91
1:K:187:ASN:O	1:K:188:VAL:HG12	1.69	0.90
1:I:255:ILE:HD12	1:I:256:GLU:H	1.35	0.90
1:K:186:SER:O	1:K:187:ASN:CB	2.19	0.90
1:A:93:GLU:HB2	1:A:96:ALA:HB2	1.53	0.90
1:E:255:ILE:HG13	1:E:256:GLU:H	1.37	0.90
1:C:108:GLN:O	1:C:109:GLU:HB2	1.70	0.88
1:A:135:CYS:SG	1:A:162:CYS:HB3	2.13	0.88
1:K:193:GLU:O	1:K:194:ALA:HB3	1.74	0.87
1:K:185:THR:HG21	1:K:193:GLU:HG3	1.55	0.86
1:G:94:ASP:O	1:G:96:ALA:N	2.07	0.86
1:E:188:VAL:O	1:E:189:ASP:CB	2.24	0.86
1:K:123:VAL:HG23	1:K:123:VAL:O	1.75	0.85
1:G:64:ARG:HH21	1:G:94:ASP:CG	1.79	0.85
1:K:187:ASN:O	1:K:188:VAL:CG1	2.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ASP:O	1:C:190:LYS:HB2	1.77	0.85
1:E:255:ILE:HG13	1:E:256:GLU:N	1.92	0.84
2:F:2:ALA:C	2:F:3:VAL:HG22	1.97	0.84
1:A:187:ASN:O	1:A:188:VAL:O	1.95	0.84
1:K:5:ARG:HB3	1:K:59:THR:HB	1.58	0.84
1:G:183:SER:OG	1:K:109:GLU:HG3	1.76	0.84
1:G:258:GLU:O	1:G:260:GLY:N	2.11	0.84
2:D:1:SER:O	2:D:2:ALA:CB	2.26	0.84
1:K:95:ASN:O	1:K:96:ALA:O	1.96	0.84
1:G:189:ASP:OD2	1:G:189:ASP:O	1.97	0.83
1:C:23[A]:ILE:HD13	1:C:39:SER:HB3	1.61	0.82
1:K:187:ASN:C	1:K:188:VAL:HG12	2.00	0.82
1:I:241:ILE:O	1:I:241:ILE:CG1	2.27	0.81
1:E:188:VAL:O	1:E:189:ASP:OD2	1.97	0.81
1:I:192:GLU:O	1:I:192:GLU:CG	2.27	0.81
1:A:95:ASN:O	1:A:96:ALA:O	1.99	0.81
1:I:110:LYS:O	1:I:110:LYS:CG	2.29	0.80
1:E:193:GLU:O	1:E:194:ALA:HB2	1.82	0.79
1:K:187:ASN:O	1:K:188:VAL:CB	2.27	0.79
2:H:1:SER:O	2:H:2:ALA:HB2	1.79	0.79
2:D:2:ALA:O	2:D:3:VAL:CG2	2.31	0.78
1:A:27:CYS:HB2	3:A:2024:HOH:O	1.82	0.78
1:A:191:GLU:HG2	3:A:2031:HOH:O	1.82	0.78
1:G:108:GLN:HE21	1:G:109:GLU:H	1.32	0.78
2:B:2:ALA:O	2:B:3:VAL:HG13	1.84	0.78
1:G:64:ARG:NH2	1:G:94:ASP:CG	2.36	0.78
1:K:186:SER:O	1:K:187:ASN:HB3	1.83	0.78
1:G:107:ASN:O	1:G:108:GLN:CB	2.31	0.78
1:G:108:GLN:NE2	1:G:109:GLU:H	1.82	0.77
1:G:255:ILE:O	2:H:4:LEU:HD12	1.85	0.77
1:I:191:GLU:O	1:I:192:GLU:CB	2.32	0.76
1:I:255:ILE:HD12	1:I:256:GLU:N	2.01	0.76
2:L:15:LYS:O	2:L:16:LYS:HB2	1.83	0.76
1:K:123:VAL:O	1:K:123:VAL:CG2	2.34	0.76
1:E:70:VAL:HG13	1:E:116:MET:CE	2.17	0.74
1:A:188:VAL:HG13	1:A:189:ASP:N	2.00	0.74
2:H:12:PHE:CD1	2:H:12:PHE:N	2.54	0.74
1:A:40:MET:SD	2:B:8:ILE:HG21	2.28	0.73
1:C:184:GLN:O	1:C:185:THR:C	2.27	0.73
1:I:64:ARG:O	1:I:66:LEU:HD12	1.89	0.73
1:K:96:ALA:O	1:K:97:ASP:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:LYS:H	1:E:199:MET:HE3	1.54	0.73
1:K:192:GLU:O	1:K:192:GLU:HG3	1.87	0.72
2:B:16:LYS:H	2:B:16:LYS:HD3	1.55	0.72
1:I:108:GLN:HG2	1:I:108:GLN:O	1.87	0.72
1:C:24[B]:ASN:H	1:C:24[B]:ASN:ND2	1.86	0.72
1:A:91:ARG:HH11	1:A:91:ARG:HB3	1.53	0.72
1:E:256:GLU:O	1:E:257:ASP:C	2.28	0.72
1:G:189:ASP:OD2	1:G:192:GLU:OE2	2.07	0.72
1:C:61:ARG:NH1	1:C:63:ASP:OD2	2.22	0.71
1:K:187:ASN:O	1:K:188:VAL:HB	1.87	0.71
1:K:187:ASN:ND2	1:K:188:VAL:N	2.38	0.71
1:E:99:LEU:HD12	1:E:100:ALA:H	1.56	0.71
1:I:9:GLY:HA3	1:I:88:ILE:HG13	1.72	0.70
1:G:164:LYS:HD2	3:G:2037:HOH:O	1.90	0.70
1:I:107:ASN:O	1:I:109:GLU:OE1	2.08	0.70
1:E:190:LYS:HD3	1:E:191:GLU:N	2.07	0.69
2:D:16:LYS:HE3	2:D:16:LYS:HA	1.74	0.69
1:I:190:LYS:CG	1:I:190:LYS:O	2.40	0.69
1:E:4:ALA:HA	1:E:59:THR:O	1.92	0.69
1:E:95:ASN:ND2	1:E:95:ASN:H	1.91	0.69
1:K:188:VAL:HG22	1:K:189:ASP:OD2	1.92	0.69
1:K:193:GLU:O	1:K:194:ALA:CB	2.39	0.69
1:A:135:CYS:SG	1:A:162:CYS:CB	2.81	0.69
1:C:139:MET:HB2	1:C:140:PRO:HD2	1.75	0.68
1:G:193:GLU:O	1:G:193:GLU:CG	2.41	0.68
1:I:107:ASN:O	1:I:109:GLU:N	2.26	0.68
1:A:121:LEU:O	1:A:122:ASP:HB3	1.94	0.68
1:G:108:GLN:O	1:G:109:GLU:CB	2.42	0.68
1:I:3:GLU:OE2	1:I:91:ARG:NE	2.26	0.68
1:G:24:ASN:ND2	1:G:24:ASN:H	1.91	0.68
1:K:163:ALA:HA	1:K:199:MET:CE	2.24	0.68
1:A:93:GLU:HB2	1:A:96:ALA:CB	2.24	0.67
1:G:233:VAL:HB	1:G:234:PRO:HD2	1.76	0.67
1:C:97:ASP:OD2	1:C:97:ASP:N	2.16	0.67
1:G:139:MET:HB2	1:G:140:PRO:HD2	1.76	0.67
1:E:257:ASP:C	1:E:257:ASP:OD1	2.32	0.67
2:F:2:ALA:O	2:F:3:VAL:CB	2.41	0.67
1:G:5:ARG:HB3	1:G:59:THR:HB	1.76	0.67
1:E:22:LEU:HD13	1:E:214:PHE:CB	2.24	0.66
1:A:210:ARG:HG3	1:A:210:ARG:HH11	1.60	0.66
1:A:242:ALA:O	1:A:243:ASP:HB2	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:SER:O	2:B:2:ALA:HB2	1.95	0.66
1:G:139:MET:HB2	1:G:140:PRO:CD	2.26	0.66
1:I:108:GLN:N	1:I:108:GLN:NE2	2.44	0.66
1:K:233:VAL:CG2	1:K:234:PRO:HD2	2.26	0.66
1:G:189:ASP:C	1:G:190:LYS:HG3	2.16	0.66
1:A:123:VAL:O	1:A:124:GLU:CB	2.44	0.66
1:A:134:SER:HB3	1:A:201:GLU:HB2	1.78	0.66
1:C:189:ASP:O	1:C:189:ASP:OD1	2.14	0.66
1:I:190:LYS:O	1:I:190:LYS:HG2	1.96	0.65
1:K:139:MET:HB3	1:K:195:VAL:HG13	1.79	0.65
1:G:85:GLU:CB	1:G:106:PRO:HG3	2.26	0.65
1:A:183:SER:O	1:E:109:GLU:HG3	1.95	0.65
1:K:186:SER:O	1:K:187:ASN:HB2	1.96	0.65
1:E:164:LYS:N	1:E:199:MET:HE3	2.11	0.65
1:E:70:VAL:HG13	1:E:116:MET:HE3	1.78	0.64
1:C:107:ASN:HD21	1:C:109:GLU:CB	2.08	0.64
1:I:126:LEU:N	1:I:126:LEU:HD23	2.13	0.64
1:K:122:ASP:O	1:K:123:VAL:HG22	1.97	0.64
1:G:210:ARG:HG3	1:G:210:ARG:HH11	1.62	0.64
1:E:164:LYS:H	1:E:199:MET:CE	2.10	0.64
1:G:159:VAL:HG22	1:G:206:THR:OG1	1.98	0.64
1:K:95:ASN:O	1:K:96:ALA:C	2.36	0.64
1:C:188:VAL:HG12	1:C:188:VAL:O	1.96	0.64
1:K:189:ASP:O	1:K:190:LYS:C	2.36	0.64
1:E:219:THR:N	1:E:220:PRO:CD	2.61	0.63
1:C:219:THR:N	1:C:220:PRO:CD	2.61	0.63
1:G:175:LEU:H	1:G:175:LEU:CD2	2.06	0.63
1:C:108:GLN:O	1:C:109:GLU:CB	2.45	0.63
1:K:8:GLN:HB3	1:K:11:ILE:HD12	1.81	0.63
1:K:219:THR:N	1:K:220:PRO:CD	2.61	0.63
1:K:187:ASN:C	1:K:187:ASN:ND2	2.52	0.63
1:C:113:ASP:HB2	3:C:2020:HOH:O	1.98	0.63
1:K:138:LYS:HG3	1:K:226:THR:HG22	1.81	0.62
2:L:15:LYS:O	2:L:16:LYS:CB	2.45	0.62
1:A:123:VAL:O	1:A:124:GLU:HB3	2.00	0.62
1:G:241:ILE:O	1:G:242:ALA:C	2.39	0.62
1:G:107:ASN:OD1	1:G:108:GLN:O	2.18	0.62
1:A:9:GLY:HA3	1:A:88:ILE:HD12	1.82	0.61
1:C:1:MET:HG2	1:C:61:ARG:NH2	2.15	0.61
1:K:168:LYS:CD	1:K:181:LYS:HD2	2.30	0.61
1:C:1:MET:N	1:C:94:ASP:OD1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:LYS:HE3	2:F:10:ASP:OD2	2.00	0.61
1:G:94:ASP:C	1:G:96:ALA:H	2.03	0.61
1:G:107:ASN:O	1:G:108:GLN:HB2	1.99	0.61
1:K:233:VAL:HG22	1:K:234:PRO:HD2	1.83	0.61
1:A:96:ALA:HB1	3:A:2018:HOH:O	2.00	0.61
1:C:139:MET:HB2	1:C:140:PRO:CD	2.31	0.61
1:G:175:LEU:HD23	1:G:175:LEU:N	2.12	0.61
1:A:27:CYS:CB	3:A:2024:HOH:O	2.44	0.60
1:C:93:GLU:HB2	1:C:96:ALA:HB2	1.83	0.60
1:K:185:THR:O	1:K:186:SER:HB3	2.00	0.60
1:K:191:GLU:O	1:K:192:GLU:C	2.38	0.60
1:I:82:ALA:HB2	1:I:103:PHE:CD2	2.37	0.60
1:I:168:LYS:HD2	1:I:179:ASN:HD21	1.65	0.60
1:K:143:GLU:OE1	1:K:146:ARG:NH1	2.34	0.60
1:E:3:GLU:OE1	1:E:91:ARG:NH1	2.35	0.60
1:A:210:ARG:HH11	1:A:210:ARG:CG	2.15	0.60
1:E:190:LYS:O	1:E:191:GLU:HB2	2.02	0.60
1:E:95:ASN:ND2	1:E:95:ASN:N	2.50	0.59
1:A:135:CYS:HG	1:A:162:CYS:CB	2.15	0.59
1:I:107:ASN:N	1:I:108:GLN:HE22	2.00	0.59
1:A:53:ARG:HG2	1:A:244:MET:O	2.03	0.59
2:B:16:LYS:HD3	2:B:16:LYS:N	2.13	0.59
1:G:2:PHE:O	1:G:91:ARG:HA	2.02	0.59
1:K:78:ILE:HG21	1:K:101:LEU:HD13	1.84	0.59
2:F:2:ALA:O	2:F:3:VAL:HG22	2.02	0.59
1:G:16:LEU:HD13	1:G:79:LEU:CD1	2.31	0.59
1:E:153:HIS:CG	3:E:2039:HOH:O	2.55	0.59
1:G:51:THR:O	1:G:245:GLY:HA3	2.03	0.59
1:E:5:ARG:HD3	3:E:2001:HOH:O	2.03	0.59
1:E:255:ILE:HG13	1:E:256:GLU:HG2	1.85	0.59
1:K:187:ASN:HD22	1:K:187:ASN:C	1.93	0.59
2:B:15:LYS:O	2:B:16:LYS:C	2.40	0.58
2:D:2:ALA:C	2:D:3:VAL:HG23	2.21	0.58
1:E:56:GLY:HA3	1:E:244:MET:HG3	1.84	0.58
1:G:94:ASP:C	1:G:96:ALA:N	2.56	0.58
1:A:40:MET:SD	2:B:8:ILE:HG22	2.42	0.58
1:A:121:LEU:O	1:A:122:ASP:CB	2.48	0.58
1:G:139:MET:CE	1:G:227:LEU:HD11	2.34	0.58
1:K:256:GLU:HG3	2:L:1:SER:N	2.19	0.58
2:F:2:ALA:C	2:F:3:VAL:CG2	2.67	0.58
1:G:243:ASP:HB2	3:G:2049:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:VAL:CG2	1:K:189:ASP:OD2	2.50	0.58
1:E:70:VAL:HG13	1:E:116:MET:HE1	1.86	0.58
1:E:186:SER:O	1:E:187:ASN:C	2.42	0.58
1:G:256:GLU:HA	2:H:2:ALA:HA	1.85	0.58
1:G:45:VAL:HG12	1:G:45:VAL:O	2.04	0.58
1:I:109:GLU:OE1	1:I:109:GLU:N	2.37	0.58
1:A:232:ASP:O	2:B:11:TYR:HE2	1.87	0.57
2:B:2:ALA:O	2:B:3:VAL:CG1	2.52	0.57
1:E:22:LEU:HD13	1:E:214:PHE:HB3	1.85	0.57
1:E:107:ASN:O	1:E:108:GLN:CB	2.50	0.57
1:I:70:VAL:HG12	1:I:72:LEU:HD23	1.86	0.57
1:G:255:ILE:HD12	1:G:256:GLU:H	1.69	0.57
1:A:146:ARG:HG2	1:A:146:ARG:HH11	1.69	0.57
1:I:34:GLY:HA2	1:I:60:TYR:CZ	2.39	0.57
1:C:47:LEU:HD23	1:C:47:LEU:C	2.25	0.57
1:G:45:VAL:O	1:G:45:VAL:CG1	2.53	0.57
1:E:82:ALA:HB2	1:E:103:PHE:CE2	2.40	0.57
1:K:12:LEU:HD21	1:K:90:LEU:HD11	1.85	0.57
1:C:24[A]:ASN:C	1:C:25[A]:GLU:HG2	2.24	0.56
1:G:205:LEU:HD21	1:G:231:ALA:HA	1.87	0.56
1:A:188:VAL:O	1:A:189:ASP:CB	2.43	0.56
1:E:189:ASP:OD1	1:E:189:ASP:C	2.33	0.56
1:G:85:GLU:HB3	1:G:106:PRO:HG3	1.86	0.56
1:K:37:LEU:HB3	1:K:50:LEU:HB3	1.88	0.56
1:K:163:ALA:C	1:K:199:MET:HG3	2.26	0.56
1:G:189:ASP:C	1:G:190:LYS:CG	2.74	0.56
1:K:87:ILE:HG22	3:K:2014:HOH:O	2.05	0.56
1:G:199:MET:CE	1:G:202:PRO:HG3	2.35	0.56
1:K:185:THR:OG1	1:K:194:ALA:HA	2.04	0.56
1:K:190:LYS:O	1:K:194:ALA:HB3	2.04	0.56
1:K:256:GLU:O	1:K:257:ASP:CB	2.47	0.56
1:K:51:THR:O	1:K:245:GLY:HA3	2.06	0.56
1:A:37:LEU:HB3	1:A:50:LEU:HB3	1.87	0.56
1:A:139:MET:HB2	1:A:140:PRO:CD	2.36	0.56
1:I:207:PHE:CZ	1:I:235:LEU:HB2	2.41	0.55
1:I:103:PHE:HB2	1:I:112:SER:HB2	1.89	0.55
1:I:256:GLU:O	1:I:257:ASP:C	2.44	0.55
1:E:16:LEU:HD13	1:E:79:LEU:HD12	1.87	0.55
1:C:255:ILE:C	1:C:256:GLU:CA	2.74	0.55
1:C:140:PRO:HB3	1:C:192:GLU:HG2	1.87	0.55
1:K:161:SER:OG	1:K:204:GLN:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:MET:SD	1:G:1:MET:N	2.75	0.55
1:A:183:SER:H	1:E:109:GLU:CG	2.20	0.55
1:E:193:GLU:O	1:E:193:GLU:HG3	2.07	0.55
1:E:193:GLU:O	1:E:194:ALA:CB	2.50	0.55
2:H:12:PHE:N	2:H:12:PHE:HD1	2.03	0.55
1:G:24:ASN:ND2	1:G:24:ASN:N	2.54	0.54
1:G:199:MET:HE2	1:G:202:PRO:HG3	1.89	0.54
1:E:107:ASN:O	1:E:108:GLN:HB2	2.06	0.54
1:G:108:GLN:C	1:G:109:GLU:CG	2.72	0.54
1:K:209:LEU:HD23	1:K:212:LEU:HD12	1.90	0.54
1:A:234:PRO:HD3	2:B:11:TYR:CD2	2.42	0.54
1:I:107:ASN:N	1:I:108:GLN:NE2	2.55	0.54
1:K:138:LYS:O	1:K:195:VAL:HA	2.08	0.54
1:K:168:LYS:HD2	1:K:181:LYS:HD2	1.90	0.54
1:C:190:LYS:HB2	1:C:190:LYS:NZ	2.23	0.54
1:E:190:LYS:HD3	1:E:190:LYS:C	2.27	0.54
1:I:1:MET:N	3:I:2001:HOH:O	2.32	0.54
1:G:107:ASN:O	1:G:108:GLN:HB3	2.07	0.54
1:E:188:VAL:O	1:E:189:ASP:HB3	2.06	0.54
1:G:2:PHE:CD1	1:G:30:ILE:HG21	2.43	0.54
1:G:184:GLN:HB2	1:G:197:ILE:HD12	1.90	0.53
1:G:214:PHE:O	1:G:217:LYS:HB2	2.07	0.53
1:K:163:ALA:HA	1:K:199:MET:HE2	1.88	0.53
1:K:189:ASP:O	1:K:191:GLU:O	2.26	0.53
1:A:40:MET:SD	2:B:8:ILE:HG23	2.46	0.53
1:C:199:MET:HE1	1:C:202:PRO:N	2.22	0.53
1:I:139:MET:HB2	1:I:140:PRO:HD2	1.91	0.53
1:K:43:SER:O	2:L:7:LYS:HE2	2.08	0.53
1:E:190:LYS:O	1:E:191:GLU:CB	2.56	0.53
1:I:167:VAL:HG22	1:I:168:LYS:N	2.24	0.53
1:C:48:VAL:HG23	1:C:249:TYR:CD1	2.44	0.53
1:E:35:VAL:HB	1:E:52:LEU:HB2	1.91	0.53
1:E:109:GLU:CD	1:E:109:GLU:H	2.13	0.53
1:G:81:CYS:SG	1:I:150:ASP:HB3	2.49	0.53
1:K:85:GLU:O	1:K:106:PRO:HG3	2.09	0.52
1:A:91:ARG:HB3	1:A:91:ARG:NH1	2.21	0.52
2:F:2:ALA:O	2:F:3:VAL:CG2	2.57	0.52
1:K:47:LEU:HB3	2:L:8:ILE:HD13	1.90	0.52
1:K:240:LYS:HZ2	1:K:246:HIS:HB3	1.75	0.52
2:H:1:SER:O	2:H:2:ALA:CB	2.47	0.52
1:A:101:LEU:N	1:A:101:LEU:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:VAL:HG13	1:K:189:ASP:N	2.25	0.52
1:A:9:GLY:CA	1:A:88:ILE:HD12	2.39	0.52
1:A:146:ARG:HH11	1:A:146:ARG:CG	2.21	0.52
1:G:13:LYS:NZ	1:G:82:ALA:O	2.32	0.52
1:A:95:ASN:O	1:A:96:ALA:C	2.47	0.52
1:E:43:SER:OG	1:E:44:HIS:N	2.41	0.52
1:A:139:MET:CE	1:A:227:LEU:HD11	2.40	0.52
1:A:183:SER:H	1:E:109:GLU:HG2	1.75	0.52
1:G:243:ASP:CB	3:G:2049:HOH:O	2.56	0.52
1:A:191:GLU:CG	3:A:2031:HOH:O	2.50	0.52
1:C:199:MET:CE	1:C:202:PRO:N	2.73	0.52
1:K:8:GLN:NE2	1:K:11:ILE:HD11	2.25	0.52
1:I:107:ASN:O	1:I:108:GLN:C	2.47	0.51
1:A:106:PRO:HB2	1:A:107:ASN:ND2	2.24	0.51
2:B:3:VAL:O	2:B:4:LEU:HD23	2.09	0.51
1:E:190:LYS:NZ	1:E:191:GLU:H	2.08	0.51
1:E:217:LYS:NZ	3:E:2048:HOH:O	2.44	0.51
1:G:16:LEU:HD21	1:G:75:MET:SD	2.51	0.51
1:E:257:ASP:HA	2:F:4:LEU:HD21	1.93	0.51
1:G:85:GLU:HB2	1:G:106:PRO:HG3	1.92	0.51
1:I:203:VAL:HG11	1:I:205:LEU:CD1	2.41	0.51
1:A:188:VAL:CG1	1:A:189:ASP:N	2.71	0.51
1:K:1:MET:CE	1:K:91:ARG:HD3	2.40	0.51
1:K:7:VAL:N	3:K:2009:HOH:O	2.39	0.51
1:K:203:VAL:CG1	1:K:205:LEU:HG	2.41	0.51
1:E:242:ALA:O	1:E:243:ASP:C	2.49	0.51
1:C:1:MET:N	1:C:63:ASP:HB2	2.26	0.50
1:C:168:LYS:HG2	3:C:2033:HOH:O	2.10	0.50
1:G:2:PHE:HB2	1:G:66:LEU:HD11	1.92	0.50
1:G:189:ASP:O	1:G:190:LYS:HG3	2.12	0.50
1:G:136:VAL:HG22	1:G:228:SER:HB2	1.93	0.50
1:K:185:THR:HG21	1:K:193:GLU:CG	2.33	0.50
1:G:34:GLY:HA2	1:G:60:TYR:CZ	2.46	0.50
1:G:206:THR:HG22	1:G:254:LYS:HB2	1.94	0.50
1:I:40:MET:HE3	1:I:44:HIS:CD2	2.47	0.50
1:K:188:VAL:HG13	1:K:189:ASP:H	1.75	0.50
1:A:206:THR:HG22	1:A:254:LYS:HB2	1.94	0.50
1:A:210:ARG:CG	1:A:210:ARG:NH1	2.74	0.50
1:C:199:MET:HE1	1:C:202:PRO:CD	2.40	0.50
1:E:190:LYS:HZ3	1:E:191:GLU:H	1.58	0.50
1:E:95:ASN:O	1:E:96:ALA:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:ASP:OD2	1:G:257:ASP:C	2.49	0.50
1:I:20:LYS:HD3	1:I:76:SER:OG	2.11	0.50
1:I:97:ASP:CB	1:I:98:THR:HG22	2.42	0.50
1:I:185:THR:O	1:I:186:SER:O	2.30	0.50
1:G:241:ILE:O	1:G:242:ALA:O	2.30	0.50
2:F:5:GLN:HG3	2:F:6:LYS:O	2.12	0.49
1:I:14:LYS:HD3	1:I:220:PRO:HB3	1.94	0.49
1:A:47:LEU:C	1:A:47:LEU:HD23	2.32	0.49
1:C:189:ASP:O	1:C:189:ASP:CG	2.49	0.49
1:E:241:ILE:O	1:E:242:ALA:C	2.50	0.49
1:E:71:ASN:HD22	1:E:119:MET:CE	2.25	0.49
1:G:183:SER:OG	1:K:109:GLU:CG	2.55	0.49
1:C:78:ILE:HG21	1:C:101:LEU:HD13	1.93	0.49
1:G:161:SER:OG	1:G:204:GLN:HG3	2.12	0.49
1:C:175:LEU:C	1:C:175:LEU:HD12	2.33	0.49
1:K:240:LYS:NZ	1:K:246:HIS:HB3	2.28	0.49
1:C:199:MET:HE2	1:C:202:PRO:HA	1.93	0.49
1:G:3:GLU:HA	1:G:90:LEU:O	2.13	0.49
1:C:25[B]:GLU:OE2	1:C:119:MET:SD	2.71	0.49
1:C:199:MET:HE2	1:C:202:PRO:CA	2.42	0.49
1:E:71:ASN:HD22	1:E:119:MET:HE1	1.77	0.49
1:G:52:LEU:HD21	1:G:241:ILE:HD13	1.93	0.49
1:I:125:GLN:C	1:I:126:LEU:HD23	2.34	0.49
1:C:256:GLU:O	1:C:257:ASP:C	2.51	0.48
1:I:168:LYS:HD2	1:I:179:ASN:ND2	2.28	0.48
1:A:185:THR:O	1:A:188:VAL:HB	2.14	0.48
1:I:34:GLY:HA2	1:I:60:TYR:OH	2.13	0.48
1:K:230:SER:O	1:K:233:VAL:HG12	2.12	0.48
2:B:16:LYS:H	2:B:16:LYS:CD	2.25	0.48
1:I:127:GLY:O	1:I:129:PRO:HD3	2.12	0.48
1:E:99:LEU:HD12	1:E:100:ALA:N	2.25	0.48
1:G:19:LEU:HD21	1:G:247:LEU:HD11	1.95	0.48
1:K:187:ASN:HD22	1:K:188:VAL:H	1.49	0.48
1:A:167:VAL:HG22	1:A:168:LYS:N	2.28	0.48
1:C:189:ASP:O	1:C:190:LYS:CB	2.50	0.48
1:I:82:ALA:HB2	1:I:103:PHE:CE2	2.48	0.48
1:A:241:ILE:O	1:A:242:ALA:C	2.51	0.48
1:C:23[B]:ILE:HG22	1:C:41:ASP:HA	1.95	0.48
1:C:70:VAL:HG12	1:C:72:LEU:HD23	1.95	0.48
1:E:41:ASP:O	1:E:42:SER:C	2.50	0.48
1:K:1:MET:HE3	1:K:91:ARG:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:LEU:C	1:K:37:LEU:HD23	2.34	0.48
1:A:241:ILE:HG13	1:A:246:HIS:HA	1.95	0.47
1:I:240:LYS:HB2	1:I:240:LYS:HE2	1.48	0.47
1:K:9:GLY:CA	1:K:88:ILE:HD12	2.44	0.47
1:K:134:SER:O	1:K:135:CYS:HB2	2.14	0.47
1:E:148:CYS:O	1:E:152:SER:HB3	2.14	0.47
1:C:190:LYS:HB2	1:C:190:LYS:HZ1	1.79	0.47
1:I:35:VAL:HB	1:I:52:LEU:HB2	1.95	0.47
1:I:103:PHE:CD1	1:I:103:PHE:N	2.80	0.47
1:I:108:GLN:O	1:I:109:GLU:C	2.53	0.47
1:G:218:ALA:O	1:G:221:LEU:HB2	2.13	0.47
1:G:232:ASP:O	2:H:11:TYR:HE2	1.97	0.47
1:A:7:VAL:HA	1:A:87:ILE:HG23	1.97	0.47
1:G:243:ASP:O	1:G:244:MET:CG	2.63	0.47
1:K:207:PHE:CZ	1:K:235:LEU:HB2	2.49	0.47
1:K:236:VAL:HG22	1:K:250:TYR:CD2	2.50	0.47
1:K:238:GLU:OE2	1:K:248:LYS:HE2	2.15	0.47
1:G:23:ILE:HG13	1:G:72:LEU:CD1	2.45	0.47
1:I:107:ASN:H	1:I:108:GLN:HE22	1.61	0.47
1:K:139:MET:HB2	1:K:140:PRO:HD2	1.95	0.47
2:H:16:LYS:HD3	2:H:16:LYS:HA	1.55	0.47
1:K:3:GLU:HA	1:K:90:LEU:O	2.15	0.47
1:K:18:ALA:HB1	1:K:218:ALA:HB2	1.95	0.47
1:E:153:HIS:CB	3:E:2039:HOH:O	2.62	0.47
1:G:225:VAL:HG22	1:G:226:THR:N	2.30	0.47
1:A:254:LYS:HB3	2:B:3:VAL:CG2	2.46	0.46
1:E:187:ASN:HB2	1:E:188:VAL:H	1.55	0.46
1:C:219:THR:N	1:C:220:PRO:HD3	2.29	0.46
1:E:16:LEU:HD13	1:E:79:LEU:CD1	2.45	0.46
1:G:92:ALA:HB2	1:G:99:LEU:HD12	1.98	0.46
1:G:119:MET:CE	1:G:121:LEU:HD21	2.45	0.46
1:G:188:VAL:HG23	1:G:189:ASP:N	2.29	0.46
1:C:140:PRO:HG3	1:C:193:GLU:HA	1.98	0.46
2:D:5:GLN:NE2	2:D:6:LYS:N	2.64	0.46
1:I:30:ILE:HD12	1:I:30:ILE:N	2.30	0.46
1:K:23:ILE:HG13	1:K:72:LEU:HD12	1.96	0.46
1:K:236:VAL:HG22	1:K:250:TYR:CE2	2.50	0.46
1:C:175:LEU:HD12	1:C:176:GLY:N	2.30	0.46
1:I:199:MET:HE3	1:I:199:MET:HB3	1.88	0.46
1:K:164:LYS:O	1:K:165:ASP:C	2.52	0.46
1:C:23[B]:ILE:HD13	1:C:39:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:GLU:HG2	1:G:119:MET:CE	2.46	0.46
1:A:199:MET:HE3	1:A:202:PRO:N	2.30	0.46
1:E:97:ASP:O	1:E:118:LEU:HB2	2.15	0.46
1:I:133:TYR:HB3	1:I:229:MET:O	2.15	0.46
1:K:191:GLU:O	1:K:192:GLU:O	2.34	0.46
1:A:232:ASP:O	2:B:11:TYR:CE2	2.69	0.46
1:G:207:PHE:CZ	1:G:235:LEU:HB2	2.51	0.46
1:K:188:VAL:HG12	3:K:2031:HOH:O	2.16	0.46
1:E:95:ASN:CG	1:E:96:ALA:H	2.19	0.46
1:G:4:ALA:HB1	1:G:57:PHE:CD2	2.51	0.46
1:K:168:LYS:HD3	1:K:181:LYS:HD2	1.98	0.46
2:B:16:LYS:HZ2	2:B:16:LYS:HB2	1.81	0.46
1:C:43:SER:O	1:C:45:VAL:HG23	2.15	0.46
1:E:7:VAL:HG23	1:E:58:ASP:CG	2.36	0.46
1:G:218:ALA:C	1:G:220:PRO:HD2	2.36	0.46
1:G:219:THR:N	1:G:220:PRO:CD	2.79	0.46
1:I:139:MET:HB2	1:I:140:PRO:CD	2.46	0.46
1:A:188:VAL:HG22	1:A:189:ASP:H	1.80	0.45
1:C:140:PRO:HG3	1:C:193:GLU:CA	2.46	0.45
1:E:190:LYS:NZ	1:E:191:GLU:N	2.64	0.45
1:E:244:MET:HE2	1:E:244:MET:HB2	1.66	0.45
1:A:10:SER:HB2	3:A:2002:HOH:O	2.15	0.45
1:C:107:ASN:C	1:C:107:ASN:HD22	2.20	0.45
1:E:98:THR:O	1:E:118:LEU:CD1	2.64	0.45
1:I:11:ILE:HD13	1:I:244:MET:HE1	1.98	0.45
1:I:23:ILE:HD13	1:I:39:SER:HB3	1.98	0.45
1:I:203:VAL:HG11	1:I:205:LEU:HD11	1.98	0.45
1:I:244:MET:HG2	1:I:244:MET:O	2.16	0.45
1:A:167:VAL:CG2	1:A:168:LYS:N	2.80	0.45
2:B:16:LYS:HB2	2:B:16:LYS:NZ	2.31	0.45
1:I:241:ILE:O	1:I:242:ALA:HB3	2.15	0.45
2:B:2:ALA:C	2:B:3:VAL:HG13	2.37	0.45
1:C:185:THR:HG23	1:C:195:VAL:O	2.16	0.45
1:G:7:VAL:HG23	1:G:58:ASP:OD2	2.16	0.45
1:E:107:ASN:O	1:E:108:GLN:HG3	2.16	0.45
1:E:166:GLY:HA2	1:E:197:ILE:HD13	1.99	0.45
1:C:24[A]:ASN:HB3	1:C:25[A]:GLU:HG2	1.99	0.45
1:G:34:GLY:HA2	1:G:60:TYR:OH	2.17	0.45
1:K:125:GLN:HE21	1:K:125:GLN:HB2	1.64	0.45
1:C:128:ILE:HA	1:C:129:PRO:HD3	1.90	0.45
1:E:190:LYS:CE	1:E:191:GLU:H	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:163:ALA:HA	1:K:199:MET:HE3	1.95	0.45
1:A:256:GLU:HB3	2:B:3:VAL:HG12	1.99	0.44
1:G:37:LEU:O	1:G:49:GLN:HA	2.17	0.44
1:I:79:LEU:HD13	1:I:79:LEU:HA	1.88	0.44
1:K:121:LEU:HD23	1:K:121:LEU:HA	1.76	0.44
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.83	0.44
2:D:5:GLN:NE2	2:D:6:LYS:O	2.50	0.44
1:E:190:LYS:CD	1:E:191:GLU:N	2.78	0.44
1:E:137:VAL:O	1:E:226:THR:HA	2.17	0.44
1:G:92:ALA:HB2	1:G:99:LEU:CD1	2.47	0.44
1:G:150:ASP:HB3	1:K:81:CYS:SG	2.57	0.44
1:I:38:GLN:HE21	1:I:38:GLN:HB2	1.58	0.44
1:I:64:ARG:O	1:I:66:LEU:CD1	2.60	0.44
1:E:54:SER:C	1:E:56:GLY:N	2.70	0.44
1:K:222:SER:OG	1:K:224:THR:O	2.36	0.44
1:A:159:VAL:HG22	1:A:206:THR:OG1	2.16	0.44
1:C:5:ARG:HB3	1:C:59:THR:HB	2.00	0.44
1:G:35:VAL:HB	1:G:52:LEU:HB2	2.00	0.44
1:K:240:LYS:NZ	3:K:2039:HOH:O	2.43	0.44
2:L:12:PHE:N	2:L:12:PHE:CD1	2.79	0.44
1:A:187:ASN:O	1:A:188:VAL:C	2.51	0.44
1:E:255:ILE:CG1	1:E:256:GLU:N	2.72	0.44
1:G:56:GLY:HA3	1:G:244:MET:HG2	1.99	0.44
1:G:243:ASP:O	1:G:244:MET:HG3	2.18	0.44
1:K:135:CYS:HA	1:K:198:GLU:O	2.18	0.44
1:I:23:ILE:HD12	1:I:26:ALA:HB2	2.00	0.44
1:K:139:MET:HB2	1:K:140:PRO:CD	2.47	0.44
1:G:23:ILE:HG13	1:G:72:LEU:HD12	2.00	0.43
1:I:140:PRO:HD3	1:I:194:ALA:O	2.18	0.43
1:I:161:SER:HB3	1:I:168:LYS:HB3	1.99	0.43
2:J:6:LYS:HD2	2:J:6:LYS:HA	1.75	0.43
1:K:140:PRO:HG3	1:K:193:GLU:H	1.83	0.43
1:A:255:ILE:HD13	1:A:255:ILE:HA	1.64	0.43
1:G:112:SER:HA	1:I:179:ASN:O	2.18	0.43
1:K:233:VAL:HG23	1:K:234:PRO:HD2	1.99	0.43
1:I:37:LEU:HB3	1:I:50:LEU:HB3	1.99	0.43
1:A:125:GLN:HE21	1:A:125:GLN:HB3	1.47	0.43
1:I:64:ARG:O	1:I:65:ASN:C	2.56	0.43
1:I:98:THR:HA	1:I:116:MET:O	2.19	0.43
1:K:128:ILE:H	1:K:128:ILE:HG12	1.65	0.43
1:A:1:MET:HB3	1:A:63:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:H3	1:C:63:ASP:HB2	1.83	0.43
1:C:243:ASP:HB3	3:C:2047:HOH:O	2.19	0.43
1:E:22:LEU:HD13	1:E:214:PHE:HB2	1.97	0.43
1:E:184:GLN:NE2	1:E:196:THR:HA	2.34	0.43
1:K:47:LEU:HB3	2:L:8:ILE:CD1	2.49	0.43
1:E:233:VAL:HB	1:E:234:PRO:CD	2.48	0.43
1:G:6:LEU:HD13	1:G:57:PHE:CD2	2.53	0.43
1:A:114:TYR:CE1	1:C:178:GLY:HA3	2.54	0.43
1:E:54:SER:O	1:E:56:GLY:N	2.51	0.43
2:H:4:LEU:HD13	2:H:4:LEU:O	2.18	0.43
1:K:47:LEU:CD1	1:K:126:LEU:HD12	2.49	0.43
1:K:219:THR:N	1:K:220:PRO:HD3	2.34	0.43
1:G:5:ARG:CB	1:G:59:THR:HB	2.44	0.43
1:I:187:ASN:C	1:I:189:ASP:N	2.71	0.43
1:K:187:ASN:C	1:K:188:VAL:CG1	2.69	0.43
1:C:175:LEU:HG	3:C:2031:HOH:O	2.19	0.42
1:A:91:ARG:NH1	1:A:91:ARG:CB	2.82	0.42
1:A:215:PHE:CD1	1:A:249:TYR:CD1	3.08	0.42
1:C:190:LYS:O	1:C:191:GLU:HB2	2.19	0.42
1:E:27:CYS:HA	1:E:68:MET:O	2.19	0.42
1:G:1:MET:HB2	1:G:2:PHE:H	1.54	0.42
1:I:234:PRO:HA	1:I:253:PRO:HD3	2.00	0.42
1:A:50:LEU:HD13	1:A:247:LEU:HD13	2.00	0.42
1:K:112:SER:HB3	1:K:114:TYR:CE1	2.54	0.42
1:A:185:THR:HG22	1:A:187:ASN:HB2	2.01	0.42
1:I:105:ALA:O	1:I:106:PRO:O	2.37	0.42
1:A:146:ARG:CG	1:A:146:ARG:NH1	2.82	0.42
1:A:219:THR:N	1:A:220:PRO:CD	2.82	0.42
2:D:16:LYS:HA	2:D:16:LYS:CE	2.46	0.42
1:I:207:PHE:CE1	1:I:235:LEU:HB2	2.55	0.42
1:K:70:VAL:HG12	1:K:71:ASN:C	2.40	0.42
1:E:256:GLU:H	1:E:256:GLU:HG2	1.58	0.42
1:A:20:LYS:HG3	1:A:21:ASP:N	2.35	0.42
1:G:6:LEU:HD13	1:G:57:PHE:CE2	2.55	0.42
1:I:204:GLN:HG2	1:I:204:GLN:O	2.19	0.42
1:A:44:HIS:N	1:A:44:HIS:CD2	2.87	0.42
1:E:40:MET:HG2	1:E:47:LEU:HD12	2.02	0.42
1:E:184:GLN:HE21	1:E:196:THR:HA	1.84	0.42
1:I:36:ASN:N	1:I:36:ASN:HD22	2.18	0.42
1:K:146:ARG:NH2	3:K:2025:HOH:O	2.52	0.42
1:A:30:ILE:HG22	1:A:62:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:MET:HB2	1:A:140:PRO:HD2	2.01	0.42
1:C:185:THR:HG23	1:C:195:VAL:N	2.35	0.42
1:I:133:TYR:CD1	1:I:133:TYR:N	2.87	0.42
1:K:192:GLU:O	1:K:193:GLU:CB	2.68	0.42
1:A:91:ARG:HG2	1:A:92:ALA:N	2.35	0.41
2:D:5:GLN:NE2	2:D:5:GLN:CA	2.81	0.41
1:I:145:ALA:HA	1:I:216:THR:HG21	2.02	0.41
1:C:30:ILE:HB	1:C:66:LEU:HB2	2.03	0.41
1:C:36:ASN:HA	1:C:50:LEU:O	2.20	0.41
1:C:161:SER:HB3	1:C:204:GLN:HG3	2.03	0.41
1:K:93:GLU:O	1:K:95:ASN:N	2.53	0.41
1:K:99:LEU:HD23	1:K:116:MET:HE2	2.02	0.41
1:A:24:ASN:CB	3:A:2006:HOH:O	2.69	0.41
1:A:158:VAL:HG22	1:A:159:VAL:N	2.34	0.41
1:E:188:VAL:C	1:E:189:ASP:CG	2.71	0.41
1:A:146:ARG:NH1	3:A:2027:HOH:O	2.53	0.41
1:G:92:ALA:O	1:G:93:GLU:O	2.38	0.41
1:K:185:THR:O	1:K:186:SER:CB	2.63	0.41
1:K:205:LEU:HD23	1:K:205:LEU:HA	1.81	0.41
1:K:240:LYS:HA	1:K:240:LYS:HD2	1.72	0.41
2:J:8:ILE:HG23	2:J:12:PHE:CD1	2.55	0.41
1:K:30:ILE:HD13	1:K:35:VAL:HG22	2.01	0.41
1:K:47:LEU:N	2:L:8:ILE:HD12	2.35	0.41
1:A:92:ALA:HB2	1:A:99:LEU:HD12	2.02	0.41
1:G:139:MET:HE2	1:G:227:LEU:HD11	2.01	0.41
1:G:255:ILE:O	2:H:4:LEU:CD1	2.64	0.41
1:I:167:VAL:CG2	1:I:168:LYS:N	2.83	0.41
1:I:186:SER:O	1:I:187:ASN:C	2.59	0.41
1:K:158:VAL:O	1:K:158:VAL:HG13	2.21	0.41
1:A:200:ASN:O	1:A:201:GLU:HG3	2.21	0.41
1:E:41:ASP:O	1:E:43:SER:O	2.39	0.41
1:G:225:VAL:HG21	1:G:237:VAL:HG12	2.03	0.41
1:I:203:VAL:CG1	1:I:205:LEU:CD1	2.99	0.41
1:G:259:GLU:H	1:G:259:GLU:HG3	1.50	0.41
1:I:19:LEU:HD23	1:I:19:LEU:HA	1.94	0.41
1:I:104:GLU:O	1:I:105:ALA:C	2.58	0.41
1:A:44:HIS:O	2:B:7:LYS:HB3	2.21	0.41
1:A:246:HIS:CD2	1:A:248:LYS:HE3	2.56	0.41
1:E:25:GLU:HG3	1:E:121:LEU:HD22	2.02	0.41
1:E:37:LEU:HB3	1:E:50:LEU:HB3	2.01	0.41
1:E:190:LYS:NZ	1:E:191:GLU:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:91:ARG:NH1	3:I:2025:HOH:O	2.53	0.41
1:I:97:ASP:C	1:I:98:THR:HG22	2.40	0.41
1:I:219:THR:HB	1:I:220:PRO:HD3	2.03	0.41
1:K:103:PHE:HB2	1:K:112:SER:HB2	2.02	0.41
1:K:237:VAL:HG12	1:K:239:TYR:CE1	2.55	0.41
1:E:146:ARG:NH2	3:E:2036:HOH:O	2.54	0.41
1:C:145:ALA:HA	1:C:216:THR:HG21	2.03	0.40
1:C:183:SER:O	1:C:185:THR:N	2.54	0.40
1:G:123:VAL:H	1:G:123:VAL:HG23	1.50	0.40
1:K:1:MET:N	1:K:94:ASP:OD2	2.40	0.40
1:K:68:MET:HB3	1:K:118:LEU:HD13	2.03	0.40
1:A:7:VAL:HG13	1:A:87:ILE:HD13	2.03	0.40
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.95	0.40
1:C:52:LEU:HB3	1:C:244:MET:CE	2.51	0.40
1:C:138:LYS:HB3	1:C:196:THR:HG23	2.04	0.40
1:C:237:VAL:HB	1:C:249:TYR:HB2	2.02	0.40
1:K:19:LEU:HD23	1:K:19:LEU:HA	1.83	0.40
1:A:240:LYS:NZ	3:A:2040:HOH:O	2.54	0.40
2:B:6:LYS:HD2	2:B:6:LYS:HA	1.95	0.40
1:A:183:SER:H	1:E:109:GLU:HG3	1.86	0.40
2:J:5:GLN:HG3	2:J:6:LYS:O	2.22	0.40
1:K:175:LEU:HD12	1:K:175:LEU:C	2.41	0.40
1:G:95:ASN:HD22	1:G:95:ASN:HA	1.53	0.40
1:K:79:LEU:HD23	1:K:79:LEU:HA	1.94	0.40

All (3) 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)
1:C:77:LYS:NZ	1:G:130:GLU:OE2[6_555]	1.42	0.78
1:E:42:SER:OG	1:G:243:ASP:OD1[6_555]	1.94	0.26
1:C:77:LYS:CE	1:G:130:GLU:OE2[6_555]	2.08	0.12

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	255/261 (98%)	236 (92%)	15 (6%)	4 (2%)	9 31
1	C	258/261 (99%)	233 (90%)	14 (5%)	11 (4%)	2 8
1	E	255/261 (98%)	229 (90%)	16 (6%)	10 (4%)	3 10
1	G	258/261 (99%)	237 (92%)	12 (5%)	9 (4%)	3 12
1	I	255/261 (98%)	236 (92%)	13 (5%)	6 (2%)	6 20
1	K	255/261 (98%)	224 (88%)	17 (7%)	14 (6%)	2 5
2	B	14/16 (88%)	9 (64%)	2 (14%)	3 (21%)	0 0
2	D	14/16 (88%)	11 (79%)	1 (7%)	2 (14%)	0 0
2	F	14/16 (88%)	10 (71%)	3 (21%)	1 (7%)	1 2
2	H	14/16 (88%)	11 (79%)	2 (14%)	1 (7%)	1 2
2	J	14/16 (88%)	11 (79%)	1 (7%)	2 (14%)	0 0
2	L	14/16 (88%)	12 (86%)	0	2 (14%)	0 0
All	All	1620/1662 (98%)	1459 (90%)	96 (6%)	65 (4%)	3 9

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ALA
1	A	188	VAL
2	B	2	ALA
1	C	24[A]	ASN
1	C	24[B]	ASN
1	C	108	GLN
1	C	185	THR
1	C	193	GLU
2	D	2	ALA
1	E	96	ALA
1	E	189	ASP
2	F	3	VAL
1	G	93	GLU
1	G	95	ASN
1	G	259	GLU
2	H	2	ALA
1	I	106	PRO
1	I	108	GLN
1	I	186	SER

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Mol	Chain	Res	Type
1	I	187	ASN
1	I	192	GLU
2	J	3	VAL
1	K	94	ASP
1	K	96	ALA
1	K	186	SER
1	K	187	ASN
1	K	188	VAL
1	K	189	ASP
1	A	124	GLU
1	A	190	LYS
2	B	3	VAL
1	C	107	ASN
1	C	184	GLN
1	C	186	SER
1	C	192	GLU
2	D	3	VAL
1	E	106	PRO
1	E	108	GLN
1	E	194	ALA
1	G	108	GLN
1	G	188	VAL
1	G	242	ALA
1	G	244	MET
1	I	96	ALA
1	K	123	VAL
1	K	135	CYS
1	K	191	GLU
1	K	192	GLU
1	K	194	ALA
2	L	2	ALA
1	C	109	GLU
1	E	65	ASN
2	J	2	ALA
1	K	165	ASP
1	K	190	LYS
1	C	190	LYS
1	E	55	GLU
1	E	187	ASN
1	E	244	MET
1	G	192	GLU
1	K	243	ASP

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Mol	Chain	Res	Type
2	L	14	PRO
2	B	14	PRO
1	E	93	GLU
1	G	241	ILE

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	225/228 (99%)	179 (80%)	46 (20%)	1	4
1	C	228/228 (100%)	175 (77%)	53 (23%)	1	2
1	E	225/228 (99%)	184 (82%)	41 (18%)	1	5
1	G	227/228 (100%)	185 (82%)	42 (18%)	1	5
1	I	225/228 (99%)	180 (80%)	45 (20%)	1	4
1	K	225/228 (99%)	180 (80%)	45 (20%)	1	4
2	B	15/15 (100%)	11 (73%)	4 (27%)	0	1
2	D	15/15 (100%)	11 (73%)	4 (27%)	0	1
2	F	15/15 (100%)	11 (73%)	4 (27%)	0	1
2	H	15/15 (100%)	11 (73%)	4 (27%)	0	1
2	J	15/15 (100%)	11 (73%)	4 (27%)	0	1
2	L	15/15 (100%)	10 (67%)	5 (33%)	0	0
All	All	1445/1458 (99%)	1148 (79%)	297 (21%)	1	3

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	ARG
1	A	24	ASN
1	A	25	GLU
1	A	32	SER
1	A	42	SER

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Mol	Chain	Res	Type
1	A	51	THR
1	A	53	ARG
1	A	64	ARG
1	A	68	MET
1	A	85	GLU
1	A	87	ILE
1	A	91	ARG
1	A	97	ASP
1	A	98	THR
1	A	104	GLU
1	A	109	GLU
1	A	125	GLN
1	A	134	SER
1	A	138	LYS
1	A	161	SER
1	A	162	CYS
1	A	164	LYS
1	A	168	LYS
1	A	181	LYS
1	A	183	SER
1	A	184	GLN
1	A	188	VAL
1	A	189	ASP
1	A	192	GLU
1	A	197	ILE
1	A	199	MET
1	A	203	VAL
1	A	204	GLN
1	A	210	ARG
1	A	217	LYS
1	A	224	THR
1	A	227	LEU
1	A	229	MET
1	A	230	SER
1	A	232	ASP
1	A	235	LEU
1	A	236	VAL
1	A	240	LYS
1	A	255	ILE
1	A	256	GLU
2	B	1	SER
2	B	8	ILE

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Mol	Chain	Res	Type
2	B	15	LYS
2	B	16	LYS
1	C	1	MET
1	C	14	LYS
1	C	16	LEU
1	C	24[A]	ASN
1	C	24[B]	ASN
1	C	25[A]	GLU
1	C	25[B]	GLU
1	C	27	CYS
1	C	32	SER
1	C	47	LEU
1	C	48	VAL
1	C	49	GLN
1	C	55	GLU
1	C	58	ASP
1	C	59	THR
1	C	61	ARG
1	C	64	ARG
1	C	68	MET
1	C	85	GLU
1	C	97	ASP
1	C	98	THR
1	C	107	ASN
1	C	108	GLN
1	C	109	GLU
1	C	119	MET
1	C	121	LEU
1	C	123	VAL
1	C	124	GLU
1	C	125	GLN
1	C	131	GLN
1	C	132	GLU
1	C	135	CYS
1	C	147	ILE
1	C	162	CYS
1	C	164	LYS
1	C	165	ASP
1	C	170	SER
1	C	174	GLU
1	C	186	SER
1	C	187	ASN

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Mol	Chain	Res	Type
1	C	188	VAL
1	C	189	ASP
1	C	190	LYS
1	C	196	THR
1	C	199	MET
1	C	203	VAL
1	C	210	ARG
1	C	224	THR
1	C	226	THR
1	C	230	SER
1	C	232	ASP
1	C	235	LEU
1	C	244	MET
2	D	4	LEU
2	D	5	GLN
2	D	7	LYS
2	D	16	LYS
1	E	1	MET
1	E	16	LEU
1	E	17	GLU
1	E	20	LYS
1	E	23	ILE
1	E	24	ASN
1	E	27	CYS
1	E	33	SER
1	E	46	SER
1	E	47	LEU
1	E	49	GLN
1	E	54	SER
1	E	66	LEU
1	E	80	LYS
1	E	93	GLU
1	E	95	ASN
1	E	97	ASP
1	E	98	THR
1	E	113	ASP
1	E	120	ASP
1	E	121	LEU
1	E	123	VAL
1	E	124	GLU
1	E	132	GLU
1	E	135	CYS

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Mol	Chain	Res	Type
1	E	154	ILE
1	E	164	LYS
1	E	181	LYS
1	E	183	SER
1	E	187	ASN
1	E	188	VAL
1	E	190	LYS
1	E	193	GLU
1	E	199	MET
1	E	217	LYS
1	E	224	THR
1	E	228	SER
1	E	229	MET
1	E	254	LYS
1	E	256	GLU
1	E	257	ASP
2	F	1	SER
2	F	4	LEU
2	F	7	LYS
2	F	16	LYS
1	G	1	MET
1	G	10	SER
1	G	16	LEU
1	G	17	GLU
1	G	20	LYS
1	G	23	ILE
1	G	24	ASN
1	G	30	ILE
1	G	39	SER
1	G	41	ASP
1	G	61	ARG
1	G	64	ARG
1	G	73	THR
1	G	97	ASP
1	G	110	LYS
1	G	113	ASP
1	G	123	VAL
1	G	130	GLU
1	G	132	GLU
1	G	135	CYS
1	G	138	LYS
1	G	156	ASP

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Mol	Chain	Res	Type
1	G	161	SER
1	G	162	CYS
1	G	175	LEU
1	G	179	ASN
1	G	186	SER
1	G	187	ASN
1	G	190	LYS
1	G	191	GLU
1	G	192	GLU
1	G	193	GLU
1	G	199	MET
1	G	206	THR
1	G	210	ARG
1	G	226	THR
1	G	227	LEU
1	G	228	SER
1	G	237	VAL
1	G	240	LYS
1	G	256	GLU
1	G	259	GLU
2	H	3	VAL
2	H	4	LEU
2	H	12	PHE
2	H	16	LYS
1	I	10	SER
1	I	16	LEU
1	I	36	ASN
1	I	38	GLN
1	I	49	GLN
1	I	61	ARG
1	I	64	ARG
1	I	79	LEU
1	I	85	GLU
1	I	98	THR
1	I	99	LEU
1	I	101	LEU
1	I	108	GLN
1	I	109	GLU
1	I	113	ASP
1	I	120	ASP
1	I	121	LEU
1	I	123	VAL

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Mol	Chain	Res	Type
1	I	124	GLU
1	I	125	GLN
1	I	131	GLN
1	I	135	CYS
1	I	179	ASN
1	I	181	LYS
1	I	185	THR
1	I	187	ASN
1	I	189	ASP
1	I	190	LYS
1	I	191	GLU
1	I	199	MET
1	I	201	GLU
1	I	217	LYS
1	I	223	SER
1	I	224	THR
1	I	226	THR
1	I	228	SER
1	I	232	ASP
1	I	233	VAL
1	I	240	LYS
1	I	241	ILE
1	I	243	ASP
1	I	244	MET
1	I	246	HIS
1	I	247	LEU
1	I	255	ILE
2	J	3	VAL
2	J	6	LYS
2	J	7	LYS
2	J	16	LYS
1	K	8	GLN
1	K	10	SER
1	K	11	ILE
1	K	12	LEU
1	K	16	LEU
1	K	20	LYS
1	K	24	ASN
1	K	25	GLU
1	K	32	SER
1	K	33	SER
1	K	36	ASN

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Mol	Chain	Res	Type
1	K	40	MET
1	K	49	GLN
1	K	66	LEU
1	K	78	ILE
1	K	85	GLU
1	K	95	ASN
1	K	98	THR
1	K	108	GLN
1	K	109	GLU
1	K	115	GLU
1	K	117	LYS
1	K	120	ASP
1	K	122	ASP
1	K	124	GLU
1	K	125	GLN
1	K	128	ILE
1	K	156	ASP
1	K	161	SER
1	K	175	LEU
1	K	181	LYS
1	K	187	ASN
1	K	189	ASP
1	K	191	GLU
1	K	195	VAL
1	K	197	ILE
1	K	199	MET
1	K	204	GLN
1	K	210	ARG
1	K	222	SER
1	K	224	THR
1	K	230	SER
1	K	232	ASP
1	K	240	LYS
1	K	256	GLU
2	L	1	SER
2	L	3	VAL
2	L	4	LEU
2	L	8	ILE
2	L	15	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	44	HIS
1	A	65	ASN
1	A	107	ASN
1	A	125	GLN
1	C	36	ASN
1	C	44	HIS
1	C	65	ASN
1	C	107	ASN
2	D	5	GLN
1	E	44	HIS
1	E	65	ASN
1	E	71	ASN
1	E	95	ASN
1	E	107	ASN
1	E	184	GLN
1	E	187	ASN
1	G	24	ASN
1	G	49	GLN
1	G	65	ASN
1	G	95	ASN
1	G	108	GLN
1	G	125	GLN
1	I	36	ASN
1	I	44	HIS
1	I	65	ASN
1	I	108	GLN
1	I	125	GLN
1	I	179	ASN
1	K	8	GLN
1	K	65	ASN
1	K	125	GLN
1	K	187	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	255:ILE	C	256:GLU	N	1.82

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	257/261 (98%)	-0.28	9 (3%)	44	34	32, 52, 102, 162	0
1	C	257/261 (98%)	-0.50	4 (1%)	72	66	28, 44, 88, 146	0
1	E	257/261 (98%)	-0.32	10 (3%)	39	29	28, 49, 95, 151	0
1	G	260/261 (99%)	-0.32	11 (4%)	36	26	33, 54, 105, 158	0
1	I	257/261 (98%)	-0.38	8 (3%)	49	39	29, 49, 95, 156	0
1	K	257/261 (98%)	-0.32	9 (3%)	44	34	38, 55, 96, 132	0
2	B	16/16 (100%)	1.38	4 (25%)	0	0	55, 68, 151, 153	0
2	D	16/16 (100%)	0.67	3 (18%)	1	1	44, 56, 119, 120	0
2	F	16/16 (100%)	0.55	3 (18%)	1	1	50, 64, 121, 124	0
2	H	16/16 (100%)	0.43	2 (12%)	3	2	44, 63, 114, 128	0
2	J	16/16 (100%)	0.50	2 (12%)	3	2	50, 67, 125, 129	0
2	L	16/16 (100%)	0.33	3 (18%)	1	1	47, 57, 114, 121	0
All	All	1641/1662 (98%)	-0.29	68 (4%)	37	27	28, 52, 104, 162	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	ASP	14.0
1	G	189	ASP	10.4
2	B	1	SER	10.1
1	E	188	VAL	9.5
1	E	189	ASP	9.5
2	D	1	SER	7.3
2	H	1	SER	7.3
1	A	190	LYS	7.2
1	A	257	ASP	7.1
2	F	1	SER	6.8
2	B	2	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
1	K	192	GLU	6.2
2	J	1	SER	6.0
1	G	188	VAL	6.0
1	I	188	VAL	6.0
2	J	2	ALA	5.7
2	B	16	LYS	5.3
1	E	187	ASN	5.2
1	C	189	ASP	5.1
1	E	107	ASN	5.1
1	I	190	LYS	5.1
1	A	188	VAL	4.9
2	F	16	LYS	4.9
1	A	186	SER	4.6
1	G	259	GLU	4.6
2	L	16	LYS	4.5
2	L	1	SER	4.5
1	C	257	ASP	4.3
1	E	257	ASP	4.2
1	G	260	GLY	4.1
2	F	2	ALA	4.0
2	D	2	ALA	4.0
1	I	187	ASN	3.8
1	C	188	VAL	3.6
1	K	97	ASP	3.6
1	G	186	SER	3.6
1	I	189	ASP	3.5
1	I	257	ASP	3.3
1	G	191	GLU	3.3
1	I	186	SER	3.3
1	G	258	GLU	3.3
1	G	95	ASN	3.2
1	C	95	ASN	3.0
1	K	187	ASN	3.0
1	K	132	GLU	2.9
1	I	132	GLU	2.9
1	K	186	SER	2.9
2	D	16	LYS	2.8
1	K	131	GLN	2.8
1	I	130	GLU	2.8
1	E	186	SER	2.8
1	E	190	LYS	2.8
1	G	107	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	15	LYS	2.5
1	E	192	GLU	2.5
2	H	16	LYS	2.5
1	E	191	GLU	2.5
1	A	164	LYS	2.4
1	G	257	ASP	2.3
1	A	191	GLU	2.3
1	K	243	ASP	2.2
1	K	188	VAL	2.2
1	E	165	ASP	2.2
2	B	4	LEU	2.1
1	K	257	ASP	2.1
1	A	192	GLU	2.1
1	G	187	ASN	2.1
1	A	97	ASP	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 monosaccharides 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.