Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 06:33 PM EDT

PDB ID	:	3DXA
Title	:	Crystal Structure of the DM1 TCR in complex with HLA-B*4405 and decamer EBV antigen
Authors	:	Archbold, J.K.; Macdonald, W.A.; Gras, S.; Rossjohn, J.
Deposited on	:	2008-07-23
Resolution	:	3.50 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:

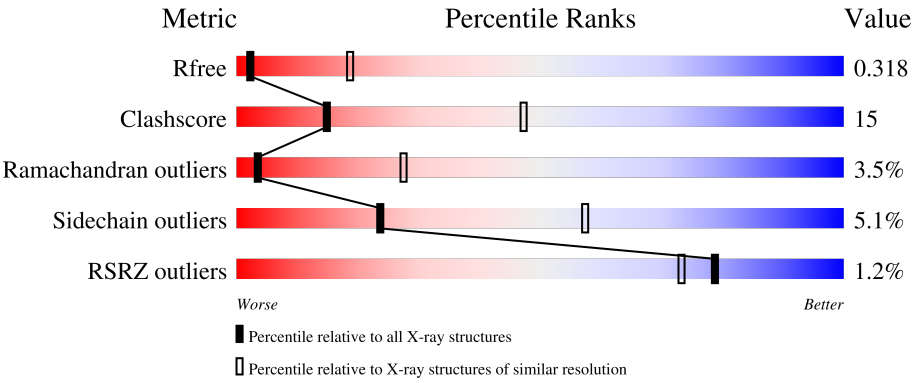
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	276	65% 29% 5% •
1	F	276	67% 27% 6%
1	K	276	5% 69% 25% 5% •
2	B	99	69% 26% 5%
2	G	99	69% 26% 5%

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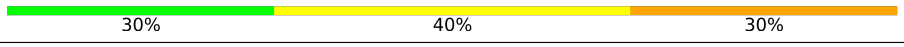
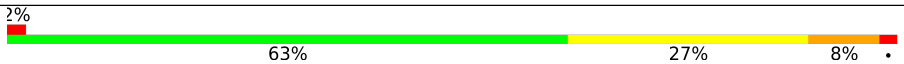
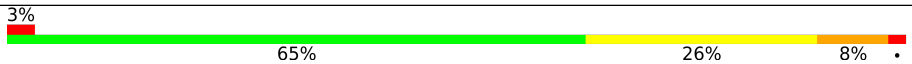
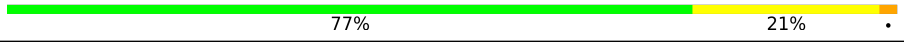
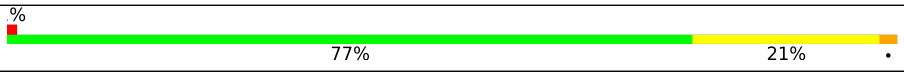
Mol	Chain	Length	Quality of chain
2	L	99	
3	C	10	
3	H	10	
3	M	10	
4	D	199	
4	I	199	
4	N	199	
5	E	244	
5	J	244	
5	O	244	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20171 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 HLA class I histocompatibility complex HLA-B*4402.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2258	1408	407	436	7			
1	F	276	Total	C	N	O	S	0	0	0
			2258	1408	407	436	7			
1	K	276	Total	C	N	O	S	0	0	0
			2258	1408	407	436	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	TYR	ASP	engineered mutation	UNP P30481
F	116	TYR	ASP	engineered mutation	UNP P30481
K	116	TYR	ASP	engineered mutation	UNP P30481

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	G	99	Total	C	N	O	S	0	1	0
			832	530	140	159	3			
2	L	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called EBV decapeptide epitope.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			91	59	14	18			
3	H	10	Total	C	N	O	0	0	0
			90	59	14	17			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	10	Total	C	N	O	0	0	0
			91	59	14	18			

- Molecule 4 is a protein called DM1 T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1560	975	262	313	10			
4	I	199	Total	C	N	O	S	0	0	0
			1560	975	262	313	10			
4	N	199	Total	C	N	O	S	0	0	0
			1560	975	262	313	10			

- Molecule 5 is a protein called DM1 T cell receptor beta chain.

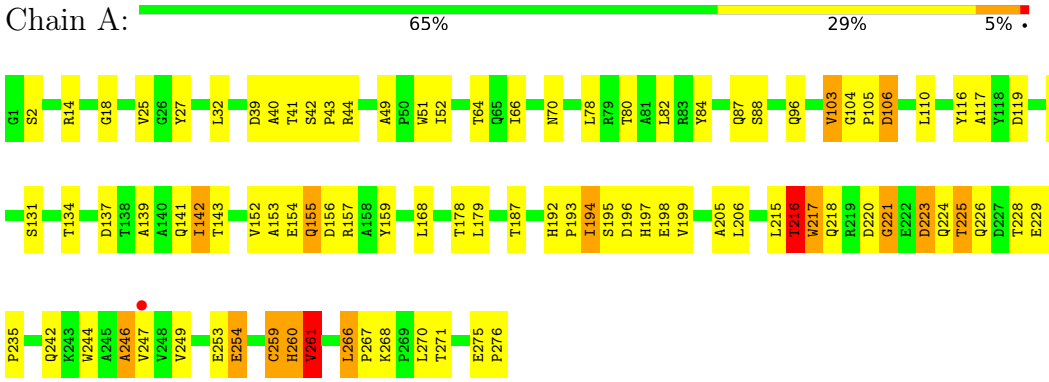
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	0	0
			1985	1244	356	379	6			
5	J	244	Total	C	N	O	S	0	0	0
			1985	1244	356	379	6			
5	O	244	Total	C	N	O	S	0	0	0
			1985	1244	356	379	6			

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.

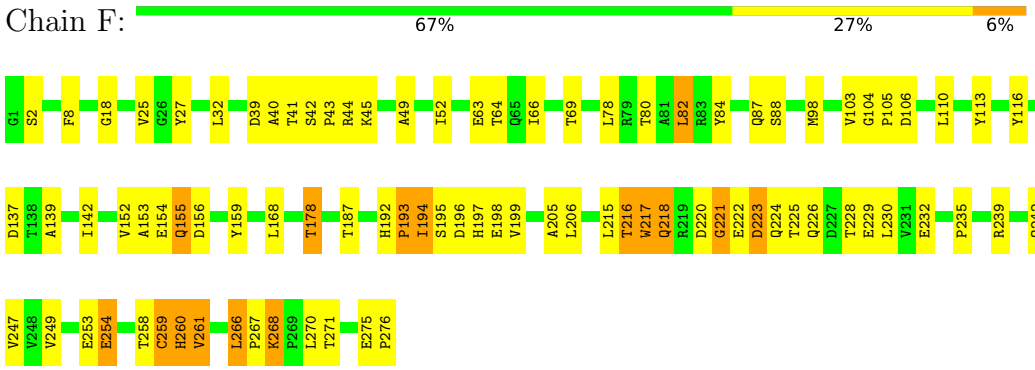
• Molecule 1: HLA class I histocompatibility complex HLA-B*4402

Chain A:



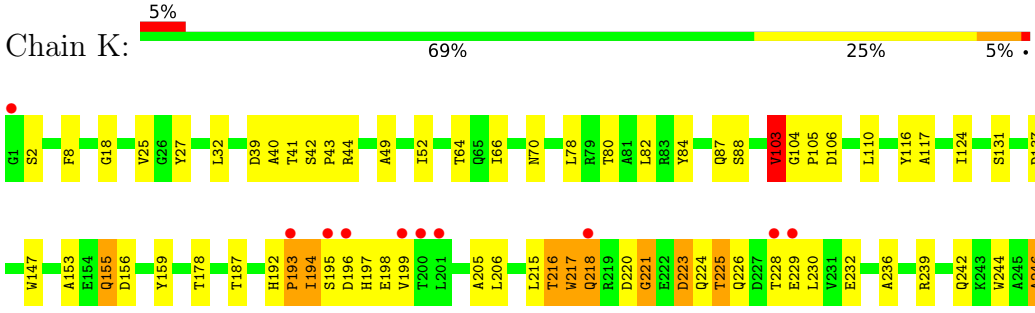
• Molecule 1: HLA class I histocompatibility complex HLA-B*4402

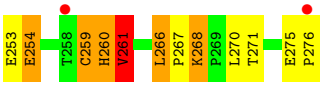
Chain F:



• Molecule 1: HLA class I histocompatibility complex HLA-B*4402

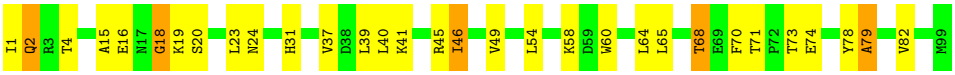
Chain K:





• Molecule 2: Beta-2-microglobulin

Chain B:

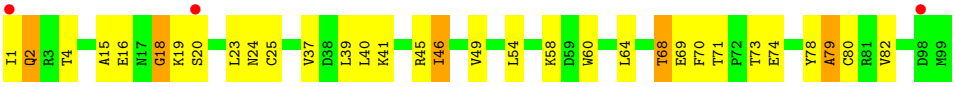


• Molecule 2: Beta-2-microglobulin

Chain G:

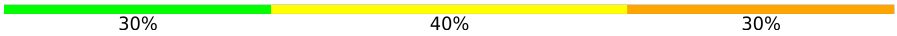
• Molecule 2: Beta-2-microglobulin

Chain L:



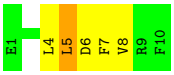
• Molecule 3: EBV decapeptide epitope

Chain C:



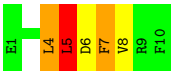
• Molecule 3: EBV decapeptide epitope

Chain H:



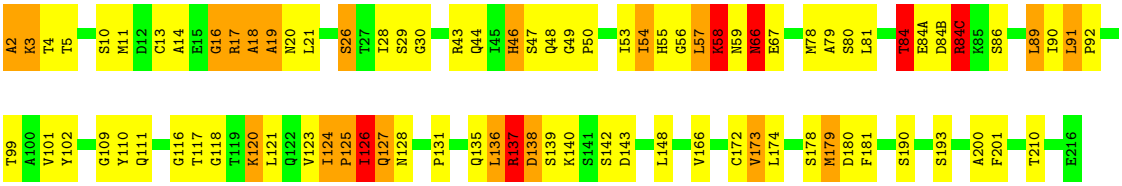
• Molecule 3: EBV decapeptide epitope

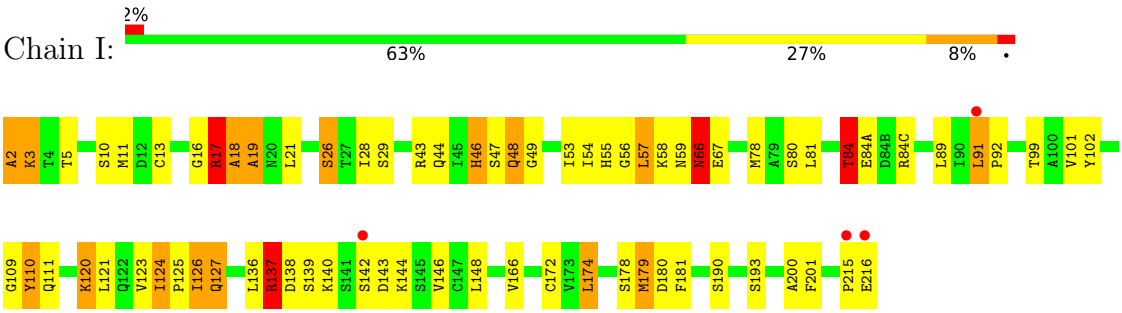
Chain M:



• Molecule 4: DM1 T cell receptor alpha chain

Chain D:



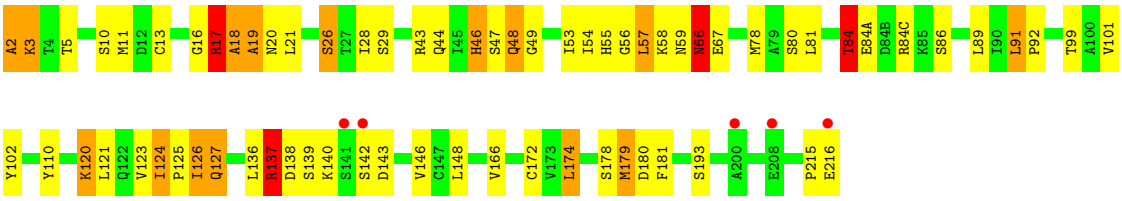


• Molecule 4: DM1 T cell receptor alpha chain

Chain I:

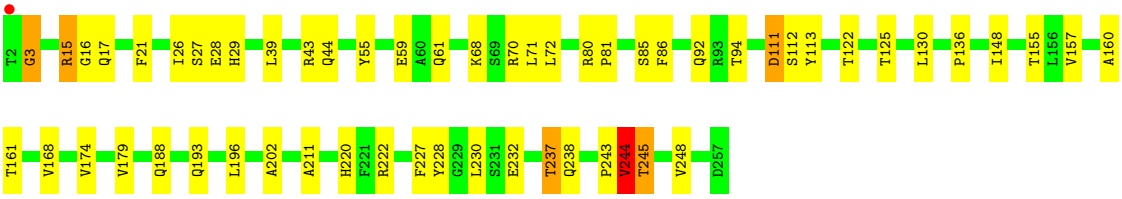
• Molecule 4: DM1 T cell receptor alpha chain

Chain N:



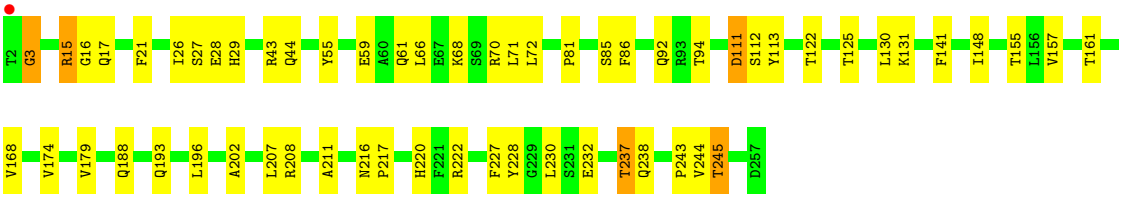
• Molecule 5: DM1 T cell receptor beta chain

Chain E:



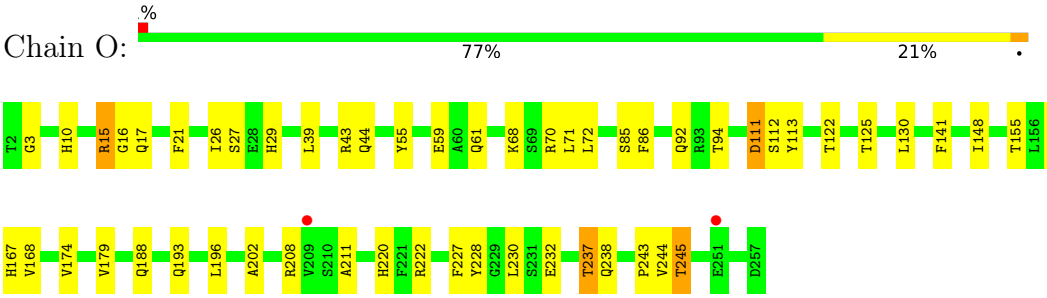
• Molecule 5: DM1 T cell receptor beta chain

Chain J:



• Molecule 5: DM1 T cell receptor beta chain

Chain O:


%
77%
21%
T2 G3 H10 R15 G16 Q17 F21 I26 S27 E28 H29 L39 R43 Q44 Y55 E59 A60 Q61 K68 S69 R70 L71 L72 S85 F86 Q92 R93 T94 D111 S112 Y113 T122 T125 L130 F141 I148 T155 L156 V157 T161
H167 V168 V174 V179 Q188 Q193 L196 A202 R208 V209 S210 A211 H220 F221 R222 F227 Y228 G229 L230 S231 E232 T237 Q238 P243 V244 T245 E251 D257

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	121.95Å 121.95Å 695.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 3.50 49.37 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (100.00-3.50) 97.5 (49.37-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.286 , 0.330 0.283 , 0.318	Depositor DCC
R_{free} test set	1970 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	73.8	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	20171	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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	0.42	0/2319	0.75	2/3154 (0.1%)
1	F	0.43	0/2319	0.65	0/3154
1	K	0.39	0/2319	0.65	1/3154 (0.0%)
2	B	0.41	0/852	0.66	0/1152
2	G	0.40	0/858	0.61	0/1160
2	L	0.36	0/852	0.58	0/1152
3	C	0.55	0/92	0.91	0/121
3	H	0.49	0/91	0.97	0/121
3	M	0.46	0/92	1.00	1/121 (0.8%)
4	D	0.50	0/1596	0.93	4/2171 (0.2%)
4	I	0.44	0/1596	0.66	0/2171
4	N	0.41	0/1596	0.68	1/2171 (0.0%)
5	E	0.43	0/2038	0.57	1/2767 (0.0%)
5	J	0.42	0/2038	0.56	0/2767
5	O	0.40	0/2038	0.55	0/2767
All	All	0.42	0/20696	0.67	10/28103 (0.0%)

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	A	0	20
1	F	0	18
1	K	0	18
2	B	0	9
2	G	0	9
2	L	0	9
4	D	0	32
4	I	0	21
4	N	0	22
All	All	0	158

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	173	VAL	CG1-CB-CG2	7.37	122.69	110.90
4	N	166	VAL	CG1-CB-CG2	7.15	122.34	110.90
5	E	244	VAL	CG1-CB-CG2	6.49	121.28	110.90
1	K	103	VAL	CG1-CB-CG2	6.48	121.27	110.90
1	A	261	VAL	CG1-CB-CG2	6.00	120.49	110.90
3	M	5	LEU	CB-CG-CD2	5.74	120.75	111.00
4	D	58	LYS	N-CA-C	5.51	125.89	111.00
4	D	136	LEU	N-CA-C	-5.38	96.48	111.00
4	D	90	ILE	N-CA-C	5.37	125.51	111.00
1	A	143	THR	N-CA-C	-5.24	96.87	111.00

There are no chirality outliers.

All (158) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	PRO	Peptide
1	A	106	ASP	Peptide
1	A	14	ARG	Peptide
1	A	142	ILE	Peptide
1	A	155	GLN	Peptide
1	A	18	GLY	Peptide
1	A	192	HIS	Peptide
1	A	194	ILE	Peptide
1	A	216	THR	Peptide
1	A	217	TRP	Peptide
1	A	218	GLN	Peptide
1	A	221	GLY	Peptide
1	A	223	ASP	Peptide
1	A	225	THR	Peptide
1	A	244	TRP	Peptide
1	A	259	CYS	Peptide
1	A	260	HIS	Peptide
1	A	266	LEU	Peptide
1	A	267	PRO	Peptide
1	A	39	ASP	Peptide
2	B	15	ALA	Peptide
2	B	16	GLU	Peptide
2	B	18	GLY	Peptide
2	B	19	LYS	Peptide
2	B	20	SER	Peptide

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Mol	Chain	Res	Type	Group
2	B	45	ARG	Peptide
2	B	68	THR	Peptide
2	B	78	TYR	Peptide
2	B	79	ALA	Peptide
4	D	10	SER	Peptide
4	D	116	GLY	Peptide
4	D	125	PRO	Peptide
4	D	127	GLN	Peptide
4	D	128	ASN	Peptide
4	D	135	GLN	Peptide
4	D	137	ARG	Peptide
4	D	16	GLY	Peptide
4	D	17	ARG	Peptide
4	D	19	ALA	Peptide
4	D	2	ALA	Peptide
4	D	20	ASN	Peptide
4	D	26	SER	Peptide
4	D	29	SER	Peptide
4	D	3	LYS	Peptide
4	D	48	GLN	Peptide
4	D	49	GLY	Peptide
4	D	50	PRO	Peptide
4	D	54	ILE	Peptide
4	D	55	HIS	Peptide
4	D	56	GLY	Peptide
4	D	57	LEU	Peptide
4	D	58	LYS	Peptide
4	D	59	ASN	Peptide
4	D	66	ASN	Peptide
4	D	67	GLU	Peptide
4	D	78	MET	Peptide
4	D	79	ALA	Peptide
4	D	84	THR	Peptide
4	D	84(C)	ARG	Peptide
4	D	89	LEU	Peptide
4	D	91	LEU	Peptide
1	F	105	PRO	Peptide
1	F	106	ASP	Peptide
1	F	155	GLN	Peptide
1	F	18	GLY	Peptide
1	F	192	HIS	Peptide
1	F	194	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	F	216	THR	Peptide
1	F	217	TRP	Peptide
1	F	218	GLN	Peptide
1	F	221	GLY	Peptide
1	F	223	ASP	Peptide
1	F	225	THR	Peptide
1	F	244	TRP	Peptide
1	F	259	CYS	Peptide
1	F	260	HIS	Peptide
1	F	266	LEU	Peptide
1	F	267	PRO	Peptide
1	F	39	ASP	Peptide
2	G	15	ALA	Peptide
2	G	16	GLU	Peptide
2	G	18	GLY	Peptide
2	G	19	LYS	Peptide
2	G	20	SER	Peptide
2	G	45	ARG	Peptide
2	G	68	THR	Peptide
2	G	78	TYR	Peptide
2	G	79	ALA	Peptide
4	I	10	SER	Peptide
4	I	127	GLN	Peptide
4	I	137	ARG	Peptide
4	I	16	GLY	Peptide
4	I	17	ARG	Peptide
4	I	19	ALA	Peptide
4	I	2	ALA	Peptide
4	I	26	SER	Peptide
4	I	29	SER	Peptide
4	I	3	LYS	Peptide
4	I	48	GLN	Peptide
4	I	49	GLY	Peptide
4	I	55	HIS	Peptide
4	I	56	GLY	Peptide
4	I	57	LEU	Peptide
4	I	59	ASN	Peptide
4	I	66	ASN	Peptide
4	I	67	GLU	Peptide
4	I	78	MET	Peptide
4	I	84	THR	Peptide
4	I	91	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	K	105	PRO	Peptide
1	K	106	ASP	Peptide
1	K	155	GLN	Peptide
1	K	18	GLY	Peptide
1	K	192	HIS	Peptide
1	K	194	ILE	Peptide
1	K	216	THR	Peptide
1	K	217	TRP	Peptide
1	K	218	GLN	Peptide
1	K	221	GLY	Peptide
1	K	223	ASP	Peptide
1	K	225	THR	Peptide
1	K	244	TRP	Peptide
1	K	259	CYS	Peptide
1	K	260	HIS	Peptide
1	K	266	LEU	Peptide
1	K	267	PRO	Peptide
1	K	39	ASP	Peptide
2	L	15	ALA	Peptide
2	L	16	GLU	Peptide
2	L	18	GLY	Peptide
2	L	19	LYS	Peptide
2	L	20	SER	Peptide
2	L	45	ARG	Peptide
2	L	68	THR	Peptide
2	L	78	TYR	Peptide
2	L	79	ALA	Peptide
4	N	10	SER	Peptide
4	N	127	GLN	Peptide
4	N	137	ARG	Peptide
4	N	16	GLY	Peptide
4	N	17	ARG	Peptide
4	N	19	ALA	Peptide
4	N	2	ALA	Peptide
4	N	20	ASN	Peptide
4	N	26	SER	Peptide
4	N	29	SER	Peptide
4	N	3	LYS	Peptide
4	N	48	GLN	Peptide
4	N	49	GLY	Peptide
4	N	55	HIS	Peptide
4	N	56	GLY	Peptide

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Mol	Chain	Res	Type	Group
4	N	57	LEU	Peptide
4	N	59	ASN	Peptide
4	N	66	ASN	Peptide
4	N	67	GLU	Peptide
4	N	78	MET	Peptide
4	N	84	THR	Peptide
4	N	91	LEU	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	2258	0	2128	85	0
1	F	2258	0	2128	82	0
1	K	2258	0	2128	73	0
2	B	829	0	794	22	0
2	G	832	0	799	21	0
2	L	829	0	794	22	0
3	C	91	0	86	15	0
3	H	90	0	86	17	0
3	M	91	0	86	10	0
4	D	1560	0	1485	63	0
4	I	1560	0	1485	56	0
4	N	1560	0	1485	52	0
5	E	1985	0	1879	46	0
5	J	1985	0	1879	49	0
5	O	1985	0	1879	44	0
All	All	20171	0	19121	596	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (596) 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)
4:N:18:ALA:CB	4:N:19:ALA:HA	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:18:ALA:CB	4:I:19:ALA:HA	1.84	1.06
1:A:246:ALA:HB3	1:A:247:VAL:HA	1.42	1.02
1:F:246:ALA:HB3	1:F:247:VAL:HA	1.40	1.01
1:K:246:ALA:HB3	1:K:247:VAL:HA	1.40	1.01
4:N:18:ALA:HB1	4:N:19:ALA:HA	1.42	1.00
4:D:18:ALA:CB	4:D:19:ALA:HA	1.94	0.98
1:F:40:ALA:HB3	1:F:41:THR:C	1.86	0.96
1:K:40:ALA:HB3	1:K:41:THR:C	1.85	0.96
4:I:18:ALA:HB1	4:I:19:ALA:HA	1.46	0.96
1:A:246:ALA:CB	1:A:247:VAL:HA	1.98	0.94
1:F:246:ALA:CB	1:F:247:VAL:HA	1.97	0.94
1:A:103:VAL:HB	1:A:104:GLY:HA2	1.50	0.93
1:A:40:ALA:HB3	1:A:41:THR:C	1.90	0.92
1:K:246:ALA:CB	1:K:247:VAL:HA	1.98	0.92
1:F:103:VAL:HB	1:F:104:GLY:HA2	1.53	0.91
1:F:66:ILE:HG23	3:H:4:LEU:HD12	1.57	0.86
1:F:155:GLN:HG3	3:H:5:LEU:HD13	1.56	0.86
5:E:220:HIS:CE1	5:J:28:GLU:OE2	2.28	0.86
2:G:18:GLY:HA2	2:G:71:THR:HG23	1.60	0.84
1:A:266:LEU:HD13	1:A:270:LEU:HD23	1.60	0.83
1:A:195:SER:N	1:A:196:ASP:HA	1.95	0.82
4:D:18:ALA:HB3	4:D:19:ALA:HA	1.60	0.82
1:K:266:LEU:HD13	1:K:270:LEU:HD23	1.62	0.81
2:L:18:GLY:HA2	2:L:71:THR:HG23	1.61	0.81
4:D:138:ASP:HB3	4:D:139:SER:HA	1.62	0.80
4:I:18:ALA:CB	4:I:19:ALA:CA	2.60	0.79
1:A:215:LEU:O	1:A:216:THR:HG23	1.83	0.79
4:I:18:ALA:HB3	4:I:19:ALA:HA	1.64	0.79
4:I:138:ASP:HB3	4:I:139:SER:HA	1.64	0.79
1:F:266:LEU:HD13	1:F:270:LEU:HD23	1.61	0.78
4:N:18:ALA:CB	4:N:19:ALA:CA	2.59	0.78
4:D:139:SER:N	4:D:140:LYS:HA	1.97	0.78
4:D:18:ALA:HB3	4:D:19:ALA:CA	2.13	0.78
1:A:217:TRP:HB2	1:A:259:CYS:HA	1.65	0.78
4:N:139:SER:N	4:N:140:LYS:HA	1.99	0.78
2:L:39:LEU:HD12	2:L:49:VAL:HG11	1.65	0.78
4:N:18:ALA:HB3	4:N:19:ALA:HA	1.66	0.78
2:B:54:LEU:HD13	2:B:64:LEU:HD21	1.66	0.77
4:D:44:GLN:HE22	5:E:44:GLN:HE22	1.32	0.77
4:N:138:ASP:HB3	4:N:139:SER:HA	1.66	0.77
2:G:39:LEU:HD12	2:G:49:VAL:HG11	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:ALA:CB	4:D:19:ALA:CA	2.64	0.76
4:D:18:ALA:HB1	4:D:19:ALA:HA	1.67	0.76
1:A:155:GLN:HG3	3:C:5:LEU:HD13	1.66	0.76
1:K:66:ILE:HG23	3:M:4:LEU:HD23	1.68	0.76
5:O:43:ARG:HD3	5:O:71:LEU:HD21	1.68	0.75
4:I:139:SER:N	4:I:140:LYS:HA	2.00	0.75
2:B:39:LEU:HD12	2:B:49:VAL:HG11	1.68	0.75
1:A:66:ILE:HG23	3:C:4:LEU:HD23	1.67	0.75
5:J:130:LEU:HD22	5:J:230:LEU:HD21	1.69	0.75
4:D:148:LEU:HD21	5:E:155:THR:HG21	1.68	0.75
1:F:215:LEU:O	1:F:216:THR:HG23	1.87	0.74
1:A:66:ILE:HG23	3:C:4:LEU:CD2	2.18	0.74
3:H:5:LEU:HD23	3:H:8:VAL:HB	1.70	0.74
2:L:49:VAL:HG13	2:L:68:THR:HB	1.68	0.74
5:E:161:THR:HG22	5:E:202:ALA:CB	2.18	0.73
1:K:215:LEU:O	1:K:216:THR:HG23	1.87	0.73
4:N:21:LEU:HD11	4:N:121:LEU:HD22	1.69	0.73
3:C:5:LEU:HD23	3:C:8:VAL:HB	1.71	0.73
1:F:217:TRP:HB2	1:F:259:CYS:HA	1.71	0.72
5:E:43:ARG:HD3	5:E:71:LEU:HD21	1.70	0.72
3:M:5:LEU:HD12	3:M:8:VAL:HB	1.72	0.72
4:D:21:LEU:HD11	4:D:121:LEU:HD22	1.71	0.71
5:E:161:THR:CG2	5:E:202:ALA:HB1	2.21	0.71
1:K:217:TRP:HB2	1:K:259:CYS:HA	1.73	0.71
5:O:161:THR:HG22	5:O:202:ALA:CB	2.20	0.71
5:O:130:LEU:HD22	5:O:230:LEU:HD21	1.72	0.71
5:O:26:ILE:HD13	5:O:29:HIS:CE1	2.26	0.70
5:O:161:THR:HG22	5:O:202:ALA:HB1	1.73	0.70
4:I:21:LEU:HD11	4:I:121:LEU:HD22	1.72	0.70
5:E:161:THR:HG22	5:E:202:ALA:HB1	1.72	0.70
5:J:43:ARG:HD3	5:J:71:LEU:HD21	1.74	0.70
5:J:161:THR:HG22	5:J:202:ALA:CB	2.22	0.70
2:G:54:LEU:HD13	2:G:64:LEU:HD21	1.72	0.70
5:E:68:LYS:HB2	5:E:72:LEU:HD12	1.75	0.69
2:G:49:VAL:HG13	2:G:68:THR:HB	1.72	0.69
2:L:54:LEU:HD13	2:L:64:LEU:HD21	1.74	0.69
4:I:148:LEU:HD21	5:J:155:THR:HG21	1.75	0.69
5:O:21:PHE:CD1	5:O:122:THR:HG21	2.27	0.69
5:J:26:ILE:HD13	5:J:29:HIS:CE1	2.28	0.69
2:B:18:GLY:HA2	2:B:71:THR:HG23	1.76	0.68
2:B:49:VAL:HG13	2:B:68:THR:HB	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:ALA:HB3	4:D:3:LYS:HG2	1.75	0.68
5:J:68:LYS:HB2	5:J:72:LEU:HD12	1.76	0.67
1:K:66:ILE:HG23	3:M:4:LEU:CD2	2.24	0.67
4:N:44:GLN:HE22	5:O:44:GLN:HE22	1.42	0.66
5:J:161:THR:HG22	5:J:202:ALA:HB1	1.75	0.66
5:O:161:THR:CG2	5:O:202:ALA:HB1	2.25	0.66
5:J:161:THR:CG2	5:J:202:ALA:HB1	2.26	0.66
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.31	0.66
1:K:78:LEU:O	1:K:82:LEU:HD23	1.96	0.66
5:E:21:PHE:CD1	5:E:122:THR:HG21	2.31	0.66
4:N:53:ILE:HG22	4:N:54:ILE:HG22	1.77	0.65
5:O:68:LYS:HB2	5:O:72:LEU:HD12	1.77	0.65
1:F:224:GLN:OE1	1:F:228:THR:HG23	1.97	0.65
4:N:43:ARG:HB2	4:N:53:ILE:HD11	1.79	0.65
1:K:103:VAL:HG13	1:K:104:GLY:HA2	1.77	0.65
4:I:43:ARG:HB2	4:I:53:ILE:HD11	1.78	0.65
1:A:82:LEU:HD13	1:A:87:GLN:HB2	1.78	0.64
1:F:246:ALA:CB	1:F:247:VAL:CA	2.74	0.64
4:I:166:VAL:HG22	4:I:190:SER:HB2	1.77	0.64
1:K:236:ALA:O	2:L:24:ASN:ND2	2.30	0.64
4:I:13:CYS:SG	4:I:19:ALA:HB2	2.36	0.64
4:D:166:VAL:HG22	4:D:190:SER:HB2	1.78	0.64
2:B:18:GLY:CA	2:B:71:THR:HG23	2.27	0.64
5:E:26:ILE:HD13	5:E:29:HIS:CE1	2.32	0.64
1:K:82:LEU:HD13	1:K:87:GLN:HB2	1.79	0.64
1:A:78:LEU:O	1:A:82:LEU:HD23	1.96	0.64
4:D:53:ILE:HG22	4:D:54:ILE:HG22	1.80	0.63
5:O:174:VAL:HG23	5:O:179:VAL:HG21	1.79	0.63
1:F:215:LEU:HD21	1:F:261:VAL:HG13	1.81	0.63
4:N:13:CYS:SG	4:N:19:ALA:HB2	2.37	0.63
5:E:130:LEU:HD22	5:E:230:LEU:HD21	1.80	0.63
1:F:82:LEU:HD13	1:F:87:GLN:HB2	1.81	0.63
1:F:78:LEU:O	1:F:82:LEU:HD23	1.98	0.63
1:A:246:ALA:CB	1:A:247:VAL:CA	2.75	0.63
5:J:21:PHE:CD1	5:J:122:THR:HG21	2.34	0.62
1:K:215:LEU:CD2	1:K:261:VAL:HG13	2.29	0.62
1:F:224:GLN:CD	1:F:228:THR:HG23	2.20	0.62
1:K:194:ILE:HG22	1:K:199:VAL:HA	1.80	0.62
1:K:215:LEU:HD21	1:K:261:VAL:HG13	1.81	0.62
1:A:84:TYR:CE1	1:A:142:ILE:HG21	2.35	0.62
4:D:43:ARG:HB2	4:D:53:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:174:VAL:HG23	5:J:179:VAL:HG21	1.82	0.62
4:D:136:LEU:HD11	5:E:157:VAL:HG21	1.82	0.62
1:K:195:SER:N	1:K:196:ASP:HA	2.16	0.61
1:A:224:GLN:OE1	1:A:228:THR:HG23	2.00	0.61
4:I:58:LYS:HZ3	4:I:84(C):ARG:HD2	1.64	0.61
3:C:4:LEU:HD12	3:C:6:ASP:HA	1.83	0.61
1:F:195:SER:N	1:F:196:ASP:HA	2.15	0.61
1:K:246:ALA:CB	1:K:247:VAL:CA	2.75	0.60
5:E:174:VAL:HG23	5:E:179:VAL:HG21	1.82	0.60
1:A:224:GLN:CD	1:A:228:THR:HG23	2.22	0.60
1:K:117:ALA:HB2	2:L:60:TRP:CE2	2.36	0.60
2:B:54:LEU:CD1	2:B:64:LEU:HD21	2.29	0.60
4:I:53:ILE:HG22	4:I:54:ILE:HG22	1.83	0.60
1:A:194:ILE:HG22	1:A:199:VAL:HA	1.84	0.60
2:G:40:LEU:H	2:G:79:ALA:HB1	1.67	0.60
1:F:103:VAL:HG22	1:F:168:LEU:HD23	1.83	0.60
5:O:10:HIS:CG	5:O:228:TYR:HB3	2.37	0.59
4:D:18:ALA:HB3	4:D:19:ALA:CB	2.31	0.59
1:F:194:ILE:HG22	1:F:199:VAL:HA	1.84	0.59
5:J:3:GLY:HA3	5:J:26:ILE:HD11	1.84	0.59
4:N:58:LYS:NZ	4:N:84(C):ARG:HD2	2.17	0.59
1:A:224:GLN:N	1:A:225:THR:HA	2.17	0.59
1:K:224:GLN:N	1:K:225:THR:HA	2.18	0.59
2:L:18:GLY:CA	2:L:71:THR:HG23	2.32	0.59
5:O:232:GLU:OE2	5:O:244:VAL:HG11	2.03	0.59
4:D:66:ASN:ND2	4:D:66:ASN:O	2.32	0.59
1:F:215:LEU:CD2	1:F:261:VAL:HG13	2.33	0.59
4:I:58:LYS:NZ	4:I:84(C):ARG:HD2	2.18	0.59
5:E:3:GLY:HA3	5:E:26:ILE:HD11	1.85	0.59
1:F:217:TRP:NE1	1:F:247:VAL:HG13	2.18	0.58
1:K:84:TYR:CE1	1:K:142:ILE:HG21	2.38	0.58
2:G:18:GLY:CA	2:G:71:THR:HG23	2.31	0.58
4:N:18:ALA:HB3	4:N:19:ALA:CA	2.29	0.58
2:G:54:LEU:CD1	2:G:64:LEU:HD21	2.34	0.58
3:M:4:LEU:HD12	3:M:6:ASP:HA	1.84	0.58
3:C:5:LEU:HB3	3:C:8:VAL:HG12	1.86	0.58
4:D:58:LYS:HZ3	4:D:84(C):ARG:HD2	1.67	0.58
4:N:139:SER:H	4:N:140:LYS:HA	1.67	0.58
4:D:13:CYS:SG	4:D:19:ALA:HB2	2.44	0.58
1:F:84:TYR:CE1	1:F:142:ILE:HG21	2.39	0.58
1:A:70:ASN:ND2	3:C:4:LEU:HD21	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:18:ALA:HB3	4:I:19:ALA:CA	2.28	0.57
5:O:43:ARG:CD	5:O:71:LEU:HD21	2.34	0.57
4:D:126:ILE:HG22	4:D:127:GLN:H	1.69	0.57
4:I:180:ASP:HB3	4:I:181:PHE:HA	1.87	0.57
1:K:224:GLN:CD	1:K:228:THR:HG23	2.24	0.57
1:A:40:ALA:HB3	1:A:42:SER:N	2.19	0.57
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.86	0.57
1:K:27:TYR:CZ	1:K:32:LEU:HD13	2.40	0.56
1:A:103:VAL:HG22	1:A:168:LEU:HD23	1.87	0.56
1:A:217:TRP:NE1	1:A:247:VAL:HG13	2.20	0.56
2:G:41:LYS:CB	2:G:46:ILE:HG23	2.36	0.56
2:L:54:LEU:CD1	2:L:64:LEU:HD21	2.35	0.56
4:N:13:CYS:SG	4:N:18:ALA:HB3	2.45	0.56
4:I:139:SER:H	4:I:140:LYS:HA	1.71	0.56
2:B:40:LEU:H	2:B:79:ALA:HB1	1.69	0.56
5:E:161:THR:HG22	5:E:202:ALA:HA	1.88	0.56
5:O:228:TYR:HA	5:O:245:THR:HG23	1.87	0.56
1:A:259:CYS:O	1:A:271:THR:HA	2.05	0.56
1:A:142:ILE:HD11	5:J:217:PRO:HG2	1.86	0.56
4:N:180:ASP:HB3	4:N:181:PHE:HA	1.88	0.56
4:D:13:CYS:SG	4:D:14:ALA:N	2.79	0.56
1:K:217:TRP:NE1	1:K:247:VAL:HG13	2.21	0.56
1:K:224:GLN:H	1:K:225:THR:HA	1.71	0.55
4:N:146:VAL:HG21	5:O:141:PHE:CE2	2.42	0.55
4:N:148:LEU:HD21	5:O:155:THR:HG21	1.88	0.55
5:E:161:THR:HG22	5:E:202:ALA:CA	2.36	0.55
1:K:224:GLN:OE1	1:K:228:THR:HG23	2.07	0.55
4:N:58:LYS:HZ3	4:N:84(C):ARG:HD2	1.72	0.55
2:B:41:LYS:CB	2:B:46:ILE:HG23	2.37	0.55
4:D:180:ASP:HB3	4:D:181:PHE:HA	1.88	0.55
5:J:228:TYR:HA	5:J:245:THR:HG23	1.87	0.55
2:L:41:LYS:CB	2:L:46:ILE:HG23	2.37	0.55
1:K:70:ASN:ND2	3:M:4:LEU:HD21	2.21	0.54
4:D:138:ASP:HB3	4:D:139:SER:CA	2.34	0.54
4:I:2:ALA:HB3	4:I:3:LYS:HG2	1.89	0.54
1:A:40:ALA:HB1	1:A:43:PRO:N	2.22	0.54
1:A:154:GLU:OE1	4:D:57:LEU:HD13	2.07	0.54
4:N:126:ILE:H	4:N:126:ILE:HD12	1.71	0.54
1:A:40:ALA:HB1	1:A:43:PRO:CA	2.37	0.54
4:D:178:SER:HB2	4:D:179:MET:HE1	1.89	0.54
1:F:40:ALA:CB	1:F:43:PRO:N	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ALA:HB2	1:A:215:LEU:HD11	1.90	0.54
1:K:247:VAL:HG23	1:K:249:VAL:HG13	1.90	0.54
1:F:40:ALA:HB1	1:F:43:PRO:N	2.23	0.54
4:N:2:ALA:HB3	4:N:3:LYS:HG2	1.89	0.54
1:A:247:VAL:HG23	1:A:249:VAL:HG13	1.90	0.53
5:J:232:GLU:OE2	5:J:244:VAL:HG11	2.08	0.53
4:N:126:ILE:HG22	4:N:127:GLN:H	1.72	0.53
1:F:27:TYR:CZ	1:F:32:LEU:HD13	2.44	0.53
1:F:205:ALA:HB2	1:F:215:LEU:HD11	1.90	0.53
3:H:5:LEU:HB3	3:H:8:VAL:HG12	1.89	0.53
1:K:40:ALA:HB3	1:K:42:SER:N	2.23	0.53
5:O:15:ARG:O	5:O:17:GLN:N	2.41	0.53
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.90	0.53
5:E:228:TYR:HA	5:E:245:THR:HG23	1.90	0.53
5:J:161:THR:HG22	5:J:202:ALA:HA	1.90	0.53
1:A:195:SER:N	1:A:196:ASP:CA	2.70	0.53
4:N:43:ARG:CB	4:N:53:ILE:HD11	2.38	0.53
1:A:253:GLU:CB	1:A:254:GLU:HA	2.39	0.53
4:D:136:LEU:HD11	5:E:157:VAL:CG2	2.37	0.53
4:D:139:SER:H	4:D:140:LYS:HA	1.68	0.53
4:D:58:LYS:NZ	4:D:84(C):ARG:HD2	2.24	0.53
1:F:103:VAL:CG2	1:F:168:LEU:HD23	2.38	0.53
1:A:253:GLU:HB2	1:A:254:GLU:HA	1.91	0.53
2:G:41:LYS:HB2	2:G:46:ILE:HG23	1.91	0.53
4:N:46:HIS:CG	4:N:47:SER:N	2.77	0.53
5:E:15:ARG:O	5:E:17:GLN:N	2.41	0.52
4:I:124:ILE:HG22	4:I:125:PRO:HD2	1.90	0.52
4:I:126:ILE:HG22	4:I:127:GLN:H	1.73	0.52
4:I:80:SER:O	4:I:89:LEU:HD12	2.09	0.52
5:J:161:THR:HG22	5:J:202:ALA:CA	2.39	0.52
5:O:26:ILE:HD12	5:O:26:ILE:H	1.75	0.52
1:A:224:GLN:H	1:A:225:THR:HA	1.74	0.52
4:D:84:THR:C	4:D:84(B):ASP:H	2.13	0.52
1:A:156:ASP:O	1:A:159:TYR:N	2.43	0.52
4:D:101:VAL:HG22	4:D:120:LYS:HG3	1.92	0.52
4:D:178:SER:HB2	4:D:179:MET:CE	2.39	0.52
1:K:40:ALA:HB1	1:K:43:PRO:N	2.25	0.52
5:E:148:ILE:HG23	5:E:211:ALA:HB1	1.90	0.52
1:F:40:ALA:HB3	1:F:42:SER:N	2.24	0.52
1:F:247:VAL:HG23	1:F:249:VAL:HG13	1.91	0.52
4:I:101:VAL:HG22	4:I:120:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:ALA:CB	1:K:43:PRO:N	2.72	0.52
1:A:40:ALA:CB	1:A:43:PRO:N	2.72	0.52
1:F:80:THR:HG22	1:F:84:TYR:CE2	2.45	0.52
4:N:58:LYS:HG3	4:N:84(C):ARG:HD3	1.92	0.52
4:N:138:ASP:HB3	4:N:139:SER:CA	2.37	0.52
2:G:40:LEU:N	2:G:79:ALA:HB1	2.25	0.52
4:I:43:ARG:CB	4:I:53:ILE:HD11	2.39	0.52
5:O:148:ILE:HG23	5:O:211:ALA:HB1	1.91	0.52
4:D:84:THR:C	4:D:84(B):ASP:N	2.63	0.51
4:I:138:ASP:HB3	4:I:139:SER:CA	2.37	0.51
5:O:26:ILE:HG22	5:O:27:SER:O	2.09	0.51
4:D:117:THR:H	4:D:118:GLY:HA2	1.76	0.51
4:I:44:GLN:HE22	5:J:44:GLN:HE22	1.57	0.51
4:D:80:SER:O	4:D:89:LEU:HD12	2.11	0.51
4:I:178:SER:HB2	4:I:179:MET:HE1	1.93	0.51
1:K:80:THR:HG22	1:K:84:TYR:CE2	2.46	0.51
4:I:126:ILE:H	4:I:126:ILE:HD12	1.75	0.51
1:K:259:CYS:O	1:K:271:THR:HA	2.10	0.51
4:D:46:HIS:CG	4:D:47:SER:N	2.77	0.51
4:I:58:LYS:HG3	4:I:84(C):ARG:HD3	1.92	0.51
1:K:253:GLU:CB	1:K:254:GLU:HA	2.40	0.51
1:A:261:VAL:O	1:A:261:VAL:HG22	2.10	0.51
1:F:253:GLU:CB	1:F:254:GLU:HA	2.41	0.51
1:K:155:GLN:HG3	3:M:5:LEU:HD23	1.93	0.51
4:D:44:GLN:HE22	5:E:44:GLN:NE2	2.06	0.51
1:A:223:ASP:HB3	1:A:224:GLN:HA	1.93	0.50
4:D:44:GLN:NE2	5:E:44:GLN:HE22	2.05	0.50
4:I:46:HIS:CG	4:I:47:SER:N	2.79	0.50
4:N:146:VAL:HG21	5:O:141:PHE:CZ	2.46	0.50
1:A:103:VAL:CG2	1:A:168:LEU:HD23	2.41	0.50
1:K:253:GLU:HB2	1:K:254:GLU:HA	1.93	0.50
4:N:124:ILE:HG22	4:N:125:PRO:HD2	1.92	0.50
5:O:21:PHE:CE1	5:O:122:THR:HG21	2.46	0.50
5:O:161:THR:HG22	5:O:202:ALA:CA	2.40	0.50
1:A:194:ILE:HG23	1:A:195:SER:OG	2.12	0.50
1:F:253:GLU:HB2	1:F:254:GLU:HA	1.94	0.50
4:N:178:SER:HB2	4:N:179:MET:CE	2.40	0.50
5:O:161:THR:HG22	5:O:202:ALA:HA	1.94	0.50
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.93	0.50
1:F:259:CYS:O	1:F:271:THR:HA	2.11	0.50
1:F:275:GLU:HB3	1:F:276:PRO:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:VAL:HG13	3:H:5:LEU:HD22	1.92	0.50
1:F:155:GLN:CG	3:H:5:LEU:HD13	2.35	0.50
1:F:187:THR:HG21	1:F:261:VAL:HG11	1.94	0.50
1:K:223:ASP:HB3	1:K:224:GLN:HA	1.93	0.50
1:K:260:HIS:N	1:K:261:VAL:HG22	2.26	0.50
5:O:168:VAL:HG12	5:O:227:PHE:HD1	1.77	0.50
1:A:96:GLN:NE2	2:B:31:HIS:NE2	2.60	0.49
1:A:229:GLU:H	1:A:246:ALA:HB3	1.77	0.49
4:D:18:ALA:HB3	4:D:19:ALA:HB2	1.94	0.49
1:K:103:VAL:CB	1:K:104:GLY:HA2	2.42	0.49
2:L:41:LYS:HB2	2:L:46:ILE:HG23	1.94	0.49
4:N:80:SER:O	4:N:89:LEU:HD12	2.12	0.49
4:D:124:ILE:HG22	4:D:125:PRO:HD2	1.94	0.49
5:E:43:ARG:CD	5:E:71:LEU:HD21	2.39	0.49
1:F:137:ASP:OD1	1:F:139:ALA:HB3	2.12	0.49
1:F:193:PRO:CB	1:F:194:ILE:HA	2.42	0.49
5:J:168:VAL:HG12	5:J:227:PHE:HD1	1.77	0.49
1:A:80:THR:HG22	1:A:84:TYR:CE2	2.48	0.49
1:A:152:VAL:HG13	3:C:5:LEU:HD22	1.95	0.49
1:K:103:VAL:HG22	1:K:104:GLY:O	2.12	0.49
1:K:205:ALA:HB2	1:K:215:LEU:HD11	1.94	0.49
2:B:41:LYS:HB2	2:B:46:ILE:HG23	1.94	0.49
4:I:58:LYS:NZ	4:I:84(C):ARG:CD	2.76	0.49
1:K:137:ASP:OD1	1:K:139:ALA:HB3	2.13	0.49
4:N:101:VAL:HG22	4:N:120:LYS:HG3	1.94	0.49
5:J:61:GLN:NE2	5:J:68:LYS:HD3	2.27	0.49
5:J:148:ILE:HG23	5:J:211:ALA:HB1	1.95	0.49
4:N:58:LYS:NZ	4:N:84(C):ARG:CD	2.74	0.49
2:B:1:ILE:HA	2:B:2:GLN:CB	2.42	0.49
1:F:156:ASP:O	1:F:159:TYR:N	2.46	0.49
3:H:8:VAL:O	3:H:8:VAL:HG13	2.13	0.49
1:A:103:VAL:HB	1:A:104:GLY:CA	2.33	0.49
1:A:275:GLU:HB3	1:A:276:PRO:C	2.33	0.49
5:E:232:GLU:OE2	5:E:244:VAL:HG21	2.12	0.49
1:F:103:VAL:HB	1:F:104:GLY:CA	2.35	0.49
4:D:131:PRO:C	4:D:210:THR:HG23	2.33	0.49
5:J:15:ARG:O	5:J:17:GLN:N	2.45	0.49
1:K:187:THR:HG21	1:K:261:VAL:HG11	1.95	0.49
1:A:155:GLN:CG	3:C:5:LEU:HD13	2.41	0.48
4:D:84:THR:O	4:D:84(B):ASP:N	2.41	0.48
4:I:178:SER:HB2	4:I:179:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:43:ARG:CD	5:J:71:LEU:HD21	2.41	0.48
2:L:1:ILE:HA	2:L:2:GLN:CB	2.43	0.48
4:N:136:LEU:HD11	5:O:157:VAL:HG21	1.95	0.48
1:A:137:ASP:OD1	1:A:139:ALA:HB3	2.14	0.48
5:E:196:LEU:N	5:E:196:LEU:HD12	2.28	0.48
1:A:27:TYR:CZ	1:A:32:LEU:HD13	2.49	0.48
1:A:217:TRP:CE3	1:A:259:CYS:HB2	2.48	0.48
5:E:21:PHE:CE1	5:E:122:THR:HG21	2.49	0.48
4:I:136:LEU:HD11	5:J:157:VAL:HG21	1.95	0.48
1:K:193:PRO:HB2	1:K:194:ILE:HA	1.95	0.48
4:D:43:ARG:CB	4:D:53:ILE:HD11	2.43	0.48
1:A:142:ILE:CD1	5:J:217:PRO:HG2	2.43	0.48
1:A:205:ALA:CB	1:A:215:LEU:HD11	2.43	0.48
5:E:161:THR:HG21	5:E:202:ALA:HB1	1.94	0.48
1:F:253:GLU:N	1:F:254:GLU:HB2	2.28	0.48
3:H:5:LEU:HD12	3:H:5:LEU:O	2.14	0.48
1:K:40:ALA:HB1	1:K:42:SER:C	2.34	0.48
1:K:103:VAL:CG1	1:K:104:GLY:HA2	2.42	0.48
1:K:275:GLU:HB3	1:K:276:PRO:C	2.34	0.48
5:O:61:GLN:NE2	5:O:68:LYS:HD3	2.29	0.48
2:B:40:LEU:N	2:B:79:ALA:HB1	2.28	0.48
5:E:61:GLN:NE2	5:E:68:LYS:HD3	2.28	0.48
1:F:2:SER:CB	1:F:104:GLY:HA3	2.43	0.48
5:J:237:THR:HG23	5:J:238:GLN:HE21	1.79	0.48
1:F:66:ILE:HA	3:H:4:LEU:HD13	1.96	0.48
1:F:205:ALA:CB	1:F:215:LEU:HD11	2.44	0.48
5:E:237:THR:HG23	5:E:238:GLN:HE21	1.79	0.48
2:G:1:ILE:HA	2:G:2:GLN:CB	2.43	0.48
1:K:268:LYS:HB2	1:K:270:LEU:HD22	1.96	0.48
5:E:112:SER:OG	5:E:113:TYR:N	2.46	0.48
1:K:2:SER:CB	1:K:104:GLY:HA3	2.44	0.48
1:K:193:PRO:CB	1:K:194:ILE:HA	2.43	0.48
5:O:161:THR:CG2	5:O:202:ALA:CB	2.89	0.47
1:F:193:PRO:HB2	1:F:194:ILE:HA	1.96	0.47
1:F:194:ILE:HG23	1:F:195:SER:OG	2.14	0.47
5:J:230:LEU:HD12	5:J:243:PRO:HD2	1.96	0.47
1:A:253:GLU:N	1:A:254:GLU:HB2	2.30	0.47
5:O:10:HIS:CD2	5:O:228:TYR:HB3	2.50	0.47
2:G:23:LEU:HD12	2:G:24:ASN:N	2.30	0.47
5:J:161:THR:CG2	5:J:202:ALA:CB	2.90	0.47
5:O:230:LEU:HD12	5:O:243:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:GLN:NE2	1:F:228:THR:HG23	2.29	0.47
3:H:4:LEU:HD23	3:H:6:ASP:HA	1.96	0.47
3:H:4:LEU:HD22	3:H:6:ASP:HB3	1.97	0.47
4:I:58:LYS:HZ3	4:I:84(C):ARG:HB3	1.79	0.47
5:J:21:PHE:CE1	5:J:122:THR:HG21	2.49	0.47
2:B:23:LEU:HD12	2:B:24:ASN:N	2.30	0.47
1:F:40:ALA:HB3	1:F:41:THR:O	2.15	0.47
4:I:137:ARG:HB3	4:I:138:ASP:HA	1.96	0.47
4:N:174:LEU:HD11	5:O:208:ARG:HD2	1.96	0.47
1:A:206:LEU:HD23	1:A:242:GLN:HG2	1.97	0.46
2:B:71:THR:HG22	2:B:73:THR:HG23	1.96	0.46
4:D:142:SER:HB2	4:D:143:ASP:HA	1.97	0.46
5:E:26:ILE:HG22	5:E:27:SER:O	2.15	0.46
1:K:229:GLU:H	1:K:246:ALA:HB3	1.80	0.46
4:N:142:SER:CB	4:N:143:ASP:HA	2.45	0.46
1:F:229:GLU:H	1:F:246:ALA:HB3	1.80	0.46
5:J:193:GLN:HB3	5:J:196:LEU:HD13	1.97	0.46
1:K:266:LEU:CD1	1:K:270:LEU:HD23	2.41	0.46
4:N:58:LYS:HZ3	4:N:84(C):ARG:HB3	1.80	0.46
1:A:25:VAL:HB	1:A:32:LEU:HD11	1.98	0.46
4:D:57:LEU:C	4:D:57:LEU:HD23	2.35	0.46
5:O:3:GLY:HA3	5:O:26:ILE:HD11	1.97	0.46
1:A:152:VAL:HG13	3:C:5:LEU:CD2	2.45	0.46
1:K:223:ASP:CB	1:K:224:GLN:HA	2.46	0.46
4:D:142:SER:CB	4:D:143:ASP:HA	2.45	0.46
1:F:25:VAL:HB	1:F:32:LEU:HD11	1.98	0.46
4:I:13:CYS:SG	4:I:18:ALA:HB3	2.55	0.46
2:L:40:LEU:H	2:L:79:ALA:HB1	1.79	0.46
4:N:142:SER:HB2	4:N:143:ASP:HA	1.97	0.46
5:O:220:HIS:HE1	5:O:222:ARG:HB2	1.81	0.46
1:A:44:ARG:HA	1:A:64:THR:HG23	1.97	0.46
1:F:69:THR:OG1	5:J:66:LEU:HD23	2.16	0.46
4:I:109:GLY:O	4:I:111:GLN:N	2.39	0.46
1:A:82:LEU:HD13	1:A:87:GLN:CB	2.44	0.46
1:A:216:THR:HG22	1:A:224:GLN:NE2	2.31	0.46
5:E:161:THR:CG2	5:E:202:ALA:CB	2.84	0.46
1:F:40:ALA:HB1	1:F:42:SER:C	2.35	0.46
1:A:116:TYR:HB2	1:A:124:ILE:HG22	1.98	0.46
1:A:119:ASP:O	2:B:1:ILE:N	2.39	0.46
1:A:123:TYR:CE2	3:C:10:PHE:CE1	3.04	0.46
5:E:230:LEU:HD12	5:E:243:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:136:LEU:O	4:D:137:ARG:HB2	2.16	0.46
4:D:138:ASP:CB	4:D:139:SER:HA	2.39	0.46
2:G:68:THR:OG1	2:G:69:GLU:N	2.49	0.46
5:O:10:HIS:HB3	5:O:167:HIS:CD2	2.51	0.46
1:A:217:TRP:HE1	1:A:247:VAL:HG13	1.81	0.45
4:D:57:LEU:C	4:D:57:LEU:CD2	2.84	0.45
1:F:218:GLN:HA	1:F:223:ASP:HB2	1.98	0.45
1:K:253:GLU:N	1:K:254:GLU:HB2	2.30	0.45
2:G:1:ILE:HA	2:G:2:GLN:HB2	1.98	0.45
5:J:220:HIS:HE1	5:J:222:ARG:HB2	1.81	0.45
5:O:112:SER:OG	5:O:113:TYR:N	2.49	0.45
4:N:58:LYS:HZ2	4:N:84(C):ARG:CD	2.30	0.45
1:A:220:ASP:N	1:A:221:GLY:HA2	2.31	0.45
5:E:39:LEU:HD23	5:E:39:LEU:C	2.37	0.45
1:K:44:ARG:HA	1:K:64:THR:HG23	1.98	0.45
2:L:1:ILE:HA	2:L:2:GLN:HB2	1.98	0.45
4:N:91:LEU:HD11	4:N:102:TYR:CE2	2.52	0.45
2:B:41:LYS:HB3	2:B:46:ILE:HG23	1.99	0.45
1:F:217:TRP:HE1	1:F:247:VAL:HG13	1.81	0.45
1:K:156:ASP:O	1:K:159:TYR:N	2.49	0.45
1:K:205:ALA:CB	1:K:215:LEU:HD11	2.46	0.45
1:A:223:ASP:CB	1:A:224:GLN:HA	2.47	0.45
4:I:166:VAL:HG22	4:I:190:SER:CB	2.44	0.45
2:L:54:LEU:HA	2:L:64:LEU:CD2	2.47	0.45
5:E:168:VAL:HG12	5:E:227:PHE:HD1	1.81	0.45
1:F:154:GLU:OE1	4:I:57:LEU:HD13	2.16	0.45
2:B:1:ILE:HA	2:B:2:GLN:HB2	1.97	0.45
4:I:142:SER:CB	4:I:143:ASP:HA	2.47	0.45
2:L:41:LYS:HB3	2:L:46:ILE:HG23	1.99	0.45
2:G:71:THR:HG22	2:G:73:THR:HG23	1.98	0.44
4:I:66:ASN:O	4:I:66:ASN:ND2	2.33	0.44
5:J:131:LYS:CB	5:J:238:GLN:HE22	2.30	0.44
2:L:40:LEU:N	2:L:79:ALA:HB1	2.32	0.44
1:F:268:LYS:HB2	1:F:270:LEU:HD22	1.98	0.44
3:H:6:ASP:O	3:H:8:VAL:N	2.50	0.44
1:K:40:ALA:HB3	1:K:41:THR:O	2.15	0.44
2:L:71:THR:HG22	2:L:73:THR:HG23	1.98	0.44
4:N:99:THR:HG22	4:N:123:VAL:H	1.83	0.44
1:A:155:GLN:NE2	3:C:3:ASN:HD21	2.16	0.44
4:D:58:LYS:HZ3	4:D:84(C):ARG:CD	2.30	0.44
1:F:155:GLN:HG3	3:H:5:LEU:CD1	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:THR:O	1:F:239:ARG:NH2	2.51	0.44
5:J:85:SER:OG	5:J:86:PHE:N	2.49	0.44
1:A:66:ILE:HG23	3:C:4:LEU:HD22	1.96	0.44
1:F:222:GLU:H	1:F:223:ASP:HA	1.82	0.44
5:E:220:HIS:HE1	5:E:222:ARG:HB2	1.83	0.44
1:K:206:LEU:HD23	1:K:242:GLN:HG2	1.99	0.44
4:N:178:SER:HB2	4:N:179:MET:HE1	1.98	0.44
2:B:54:LEU:HA	2:B:64:LEU:CD2	2.48	0.44
1:F:216:THR:HG22	1:F:224:GLN:NE2	2.33	0.44
1:K:147:TRP:CE2	3:M:8:VAL:HG23	2.53	0.44
1:F:82:LEU:HD13	1:F:87:GLN:CB	2.46	0.44
1:A:49:ALA:O	1:A:52:ILE:HG22	2.18	0.44
1:F:116:TYR:HB2	1:F:124:ILE:HG22	1.99	0.44
3:H:4:LEU:HB3	4:I:110:TYR:CD2	2.53	0.44
4:I:99:THR:HG22	4:I:123:VAL:HG23	1.99	0.44
4:N:215:PRO:O	4:N:216:GLU:C	2.55	0.44
1:A:2:SER:CB	1:A:104:GLY:HA3	2.48	0.43
4:D:30:GLY:HA2	4:D:58:LYS:NZ	2.33	0.43
5:E:28:GLU:OE2	5:J:220:HIS:CE1	2.71	0.43
4:I:136:LEU:O	4:I:137:ARG:HB2	2.18	0.43
2:L:37:VAL:HG22	2:L:82:VAL:HG22	1.99	0.43
4:N:137:ARG:HB3	4:N:138:ASP:HA	1.99	0.43
4:D:21:LEU:CD1	4:D:121:LEU:HD22	2.46	0.43
1:F:152:VAL:HG13	3:H:5:LEU:CD2	2.48	0.43
2:G:41:LYS:HB3	2:G:46:ILE:HG23	1.99	0.43
4:I:142:SER:HB2	4:I:143:ASP:HA	2.00	0.43
5:O:111:ASP:N	5:O:112:SER:HA	2.33	0.43
4:D:58:LYS:NZ	4:D:84(C):ARG:CD	2.80	0.43
1:F:220:ASP:N	1:F:221:GLY:CA	2.81	0.43
1:K:25:VAL:HB	1:K:32:LEU:HD11	2.00	0.43
1:K:216:THR:HG22	1:K:224:GLN:NE2	2.32	0.43
3:M:8:VAL:O	3:M:8:VAL:HG13	2.17	0.43
1:F:206:LEU:HD23	1:F:242:GLN:HG2	1.99	0.43
2:G:37:VAL:HG22	2:G:82:VAL:HG22	2.00	0.43
5:J:196:LEU:N	5:J:196:LEU:HD12	2.34	0.43
1:K:217:TRP:HE1	1:K:247:VAL:HG13	1.83	0.43
2:L:68:THR:OG1	2:L:69:GLU:N	2.50	0.43
4:N:18:ALA:HB3	4:N:19:ALA:CB	2.48	0.43
2:G:39:LEU:HD13	2:G:68:THR:HG22	2.01	0.43
3:M:5:LEU:HB3	3:M:8:VAL:HG12	2.00	0.43
5:J:26:ILE:HG22	5:J:27:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:39:LEU:HD23	5:O:39:LEU:C	2.39	0.43
1:A:195:SER:H	1:A:196:ASP:HA	1.78	0.43
1:A:51:TRP:CE2	1:A:179:LEU:HD11	2.54	0.43
5:J:111:ASP:N	5:J:112:SER:HA	2.34	0.43
5:O:85:SER:OG	5:O:86:PHE:N	2.52	0.43
1:F:40:ALA:HB1	1:F:43:PRO:CA	2.49	0.42
1:F:44:ARG:HA	1:F:64:THR:HG23	2.01	0.42
1:F:98:MET:HE1	1:F:113:TYR:CD2	2.53	0.42
4:I:91:LEU:HD11	4:I:102:TYR:CE2	2.54	0.42
5:O:26:ILE:O	5:O:29:HIS:HB2	2.19	0.42
3:C:5:LEU:HD12	3:C:5:LEU:O	2.18	0.42
1:K:116:TYR:HB2	1:K:124:ILE:HG22	2.00	0.42
5:O:193:GLN:HB3	5:O:196:LEU:HD13	2.00	0.42
4:D:91:LEU:HD11	4:D:102:TYR:CE2	2.54	0.42
5:E:193:GLN:HB3	5:E:196:LEU:HD13	2.01	0.42
1:F:229:GLU:H	1:F:246:ALA:CB	2.32	0.42
1:F:228:THR:HB	1:F:229:GLU:HA	2.02	0.42
1:F:235:PRO:HG2	2:G:65:LEU:HD22	2.02	0.42
4:I:99:THR:HG22	4:I:123:VAL:H	1.85	0.42
4:D:84:THR:HG21	4:D:86:SER:OG	2.20	0.42
4:D:99:THR:HG22	4:D:123:VAL:H	1.85	0.42
1:K:49:ALA:O	1:K:52:ILE:HG22	2.19	0.42
4:N:136:LEU:HD11	5:O:157:VAL:CG2	2.50	0.42
3:H:5:LEU:O	4:I:109:GLY:HA3	2.20	0.42
1:K:218:GLN:HA	1:K:223:ASP:HB2	2.02	0.42
2:L:23:LEU:HD12	2:L:24:ASN:N	2.35	0.42
1:A:96:GLN:HE22	2:B:31:HIS:CD2	2.38	0.42
1:A:156:ASP:O	1:A:157:ARG:C	2.57	0.42
1:A:229:GLU:H	1:A:246:ALA:CB	2.33	0.42
4:D:200:ALA:HB3	4:D:201:PHE:CD2	2.54	0.42
5:E:111:ASP:N	5:E:112:SER:HA	2.34	0.42
2:G:54:LEU:HA	2:G:64:LEU:CD2	2.49	0.42
1:K:40:ALA:CB	1:K:41:THR:C	2.72	0.42
4:N:124:ILE:HG22	4:N:125:PRO:CD	2.49	0.42
4:I:148:LEU:HD21	5:J:155:THR:CG2	2.48	0.42
5:O:161:THR:HG21	5:O:202:ALA:HB1	2.00	0.42
1:A:141:GLN:O	1:A:142:ILE:C	2.58	0.42
5:E:26:ILE:HD12	5:E:26:ILE:H	1.84	0.42
4:I:200:ALA:HB3	4:I:201:PHE:CD2	2.55	0.42
5:J:26:ILE:O	5:J:29:HIS:HB2	2.19	0.42
4:I:215:PRO:C	4:I:216:GLU:HG2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:112:SER:OG	5:J:113:TYR:N	2.51	0.42
3:M:6:ASP:OD1	3:M:7:PHE:N	2.53	0.42
5:O:237:THR:HG23	5:O:238:GLN:HE21	1.84	0.41
1:A:127:ASN:OD1	1:A:134:THR:OG1	2.31	0.41
1:A:224:GLN:NE2	1:A:228:THR:HG23	2.35	0.41
4:I:174:LEU:HD11	5:J:208:ARG:HD2	2.02	0.41
1:K:82:LEU:HD13	1:K:87:GLN:CB	2.47	0.41
4:N:21:LEU:CD1	4:N:121:LEU:HD22	2.46	0.41
1:A:228:THR:HB	1:A:229:GLU:HA	2.01	0.41
1:K:8:PHE:HB2	1:K:25:VAL:HG23	2.02	0.41
1:K:220:ASP:N	1:K:221:GLY:CA	2.83	0.41
4:D:166:VAL:HG22	4:D:190:SER:CB	2.47	0.41
5:E:72:LEU:HD23	5:E:72:LEU:HA	1.96	0.41
1:F:69:THR:HA	5:J:66:LEU:HD21	2.02	0.41
1:K:229:GLU:H	1:K:246:ALA:CB	2.34	0.41
4:N:66:ASN:O	4:N:66:ASN:ND2	2.37	0.41
4:N:136:LEU:O	4:N:137:ARG:HB2	2.21	0.41
4:D:99:THR:HG22	4:D:123:VAL:HG23	2.03	0.41
5:E:26:ILE:O	5:E:29:HIS:HB2	2.20	0.41
1:F:228:THR:HG22	1:F:229:GLU:N	2.36	0.41
4:I:136:LEU:HD11	5:J:157:VAL:CG2	2.51	0.41
5:J:26:ILE:H	5:J:26:ILE:HD12	1.85	0.41
1:A:40:ALA:N	1:A:41:THR:HA	2.36	0.41
1:A:266:LEU:CD1	1:A:270:LEU:HD23	2.41	0.41
4:I:143:ASP:HB2	4:I:144:LYS:CB	2.50	0.41
5:E:80:ARG:HG3	5:E:86:PHE:O	2.21	0.41
1:F:45:LYS:NZ	1:F:63:GLU:OE1	2.43	0.41
1:F:52:ILE:HD12	1:F:52:ILE:HA	1.89	0.41
1:F:217:TRP:HE3	1:F:258:THR:C	2.23	0.41
1:K:131:SER:HA	1:K:153:ALA:HB1	2.01	0.41
2:L:25:CYS:HB2	2:L:39:LEU:HD21	2.02	0.41
5:O:196:LEU:N	5:O:196:LEU:HD12	2.35	0.41
4:D:109:GLY:O	4:D:111:GLN:N	2.43	0.41
4:D:131:PRO:HB2	4:D:210:THR:HG23	2.03	0.41
5:E:160:ALA:C	5:E:161:THR:HG23	2.41	0.41
1:F:40:ALA:HB2	1:F:43:PRO:HB3	2.02	0.41
4:I:18:ALA:HB3	4:I:19:ALA:CB	2.50	0.41
5:J:161:THR:HG21	5:J:202:ALA:HB1	2.00	0.41
4:N:180:ASP:N	4:N:181:PHE:HB2	2.36	0.41
1:A:228:THR:HG22	1:A:229:GLU:N	2.36	0.41
4:D:180:ASP:N	4:D:181:PHE:HB2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:146:VAL:HG21	5:J:141:PHE:CE2	2.56	0.41
4:I:180:ASP:CB	4:I:181:PHE:HA	2.49	0.41
1:A:131:SER:HA	1:A:153:ALA:HB1	2.03	0.40
4:D:58:LYS:HG3	4:D:84(C):ARG:HD3	2.02	0.40
5:E:85:SER:OG	5:E:86:PHE:N	2.53	0.40
5:E:136:PRO:O	5:E:248:VAL:HG21	2.21	0.40
1:F:8:PHE:HB2	1:F:25:VAL:HG23	2.03	0.40
1:F:49:ALA:O	1:F:52:ILE:HG22	2.22	0.40
1:F:66:ILE:HA	3:H:4:LEU:CD1	2.51	0.40
1:F:131:SER:HA	1:F:153:ALA:HB1	2.03	0.40
2:G:39:LEU:CD1	2:G:68:THR:HG22	2.51	0.40
1:F:40:ALA:CB	1:F:41:THR:C	2.73	0.40
1:K:194:ILE:HG23	1:K:195:SER:OG	2.21	0.40
1:K:228:THR:HB	1:K:229:GLU:HA	2.02	0.40
4:N:99:THR:HG22	4:N:123:VAL:HG23	2.03	0.40
5:J:207:LEU:HD22	5:J:208:ARG:N	2.36	0.40
5:J:216:ASN:HA	5:J:217:PRO:HD3	1.98	0.40
4:N:84:THR:HG21	4:N:86:SER:OG	2.22	0.40
3:C:6:ASP:OD1	3:C:7:PHE:N	2.54	0.40
4:D:139:SER:N	4:D:140:LYS:CA	2.79	0.40
2:L:39:LEU:HD13	2:L:68:THR:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	274/276 (99%)	229 (84%)	35 (13%)	10 (4%)	3 26
1	F	274/276 (99%)	234 (85%)	33 (12%)	7 (3%)	5 33
1	K	274/276 (99%)	232 (85%)	34 (12%)	8 (3%)	4 31
2	B	97/99 (98%)	83 (86%)	13 (13%)	1 (1%)	15 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	G	98/99 (99%)	84 (86%)	13 (13%)	1 (1%)	15 54
2	L	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	15 54
3	C	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0 5
3	H	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0 5
3	M	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0 5
4	D	197/199 (99%)	149 (76%)	33 (17%)	15 (8%)	1 10
4	I	197/199 (99%)	150 (76%)	34 (17%)	13 (7%)	1 13
4	N	197/199 (99%)	151 (77%)	33 (17%)	13 (7%)	1 13
5	E	242/244 (99%)	217 (90%)	20 (8%)	5 (2%)	7 38
5	J	242/244 (99%)	218 (90%)	19 (8%)	5 (2%)	7 38
5	O	242/244 (99%)	216 (89%)	23 (10%)	3 (1%)	13 50
All	All	2455/2484 (99%)	2065 (84%)	305 (12%)	85 (4%)	3 27

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	GLU
1	A	246	ALA
4	D	11	MET
4	D	17	ARG
4	D	18	ALA
4	D	84(A)	GLU
1	F	198	GLU
1	F	246	ALA
2	G	46	ILE
4	I	18	ALA
1	K	198	GLU
1	K	246	ALA
2	L	46	ILE
4	N	18	ALA
1	A	226	GLN
1	A	260	HIS
1	A	261	VAL
2	B	46	ILE
3	C	7	PHE
4	D	46	HIS
4	D	84(C)	ARG
4	D	137	ARG

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Mol	Chain	Res	Type
4	D	138	ASP
4	D	179	MET
1	F	226	GLN
1	F	268	LYS
3	H	7	PHE
4	I	11	MET
4	I	46	HIS
4	I	137	ARG
5	J	3	GLY
1	K	226	GLN
3	M	7	PHE
4	N	11	MET
4	N	46	HIS
4	N	137	ARG
1	A	268	LYS
4	D	92	PRO
4	D	126	ILE
5	E	3	GLY
5	E	15	ARG
4	I	17	ARG
4	I	48	GLN
4	I	84(A)	GLU
4	I	110	TYR
4	I	179	MET
5	J	15	ARG
1	K	268	LYS
4	N	48	GLN
4	N	84(A)	GLU
4	N	179	MET
5	O	15	ARG
5	O	245	THR
4	D	4	THR
4	D	28	ILE
4	D	110	TYR
5	E	245	THR
1	F	254	GLU
4	N	17	ARG
4	N	110	TYR
1	A	216	THR
1	A	254	GLU
4	I	92	PRO
1	K	254	GLU

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Mol	Chain	Res	Type
4	N	28	ILE
4	N	66	ASN
4	N	92	PRO
4	I	28	ILE
4	I	66	ASN
4	I	84	THR
5	J	245	THR
4	N	84	THR
5	O	16	GLY
1	A	193	PRO
1	K	193	PRO
1	K	261	VAL
1	F	261	VAL
1	A	103	VAL
5	E	16	GLY
5	J	16	GLY
5	J	81	PRO
1	K	103	VAL
4	D	16	GLY
5	E	81	PRO
1	F	193	PRO

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	237/237 (100%)	229 (97%)	8 (3%)	37 68
1	F	237/237 (100%)	229 (97%)	8 (3%)	37 68
1	K	237/237 (100%)	228 (96%)	9 (4%)	33 65
2	B	94/94 (100%)	89 (95%)	5 (5%)	22 55
2	G	95/94 (101%)	89 (94%)	6 (6%)	18 51
2	L	94/94 (100%)	88 (94%)	6 (6%)	17 50
3	C	10/10 (100%)	8 (80%)	2 (20%)	1 7
3	H	10/10 (100%)	9 (90%)	1 (10%)	7 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	M	10/10 (100%)	8 (80%)	2 (20%)	1 7
4	D	178/178 (100%)	166 (93%)	12 (7%)	16 48
4	I	178/178 (100%)	166 (93%)	12 (7%)	16 48
4	N	178/178 (100%)	165 (93%)	13 (7%)	14 45
5	E	216/216 (100%)	206 (95%)	10 (5%)	27 61
5	J	216/216 (100%)	207 (96%)	9 (4%)	30 63
5	O	216/216 (100%)	207 (96%)	9 (4%)	30 63
All	All	2206/2205 (100%)	2094 (95%)	112 (5%)	24 57

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	SER
1	A	106	ASP
1	A	110	LEU
1	A	178	THR
1	A	197	HIS
1	A	230	LEU
1	A	232	GLU
1	A	261	VAL
2	B	2	GLN
2	B	4	THR
2	B	58	LYS
2	B	70	PHE
2	B	74	GLU
3	C	4	LEU
3	C	5	LEU
4	D	5	THR
4	D	26	SER
4	D	66	ASN
4	D	81	LEU
4	D	84	THR
4	D	120	LYS
4	D	124	ILE
4	D	126	ILE
4	D	172	CYS
4	D	173	VAL
4	D	174	LEU
4	D	193	SER
5	E	55	TYR

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Mol	Chain	Res	Type
5	E	59	GLU
5	E	70	ARG
5	E	92	GLN
5	E	94	THR
5	E	111	ASP
5	E	125	THR
5	E	188	GLN
5	E	237	THR
5	E	244	VAL
1	F	82	LEU
1	F	88	SER
1	F	110	LEU
1	F	178	THR
1	F	197	HIS
1	F	230	LEU
1	F	232	GLU
1	F	260	HIS
2	G	2	GLN
2	G	4	THR
2	G	58	LYS
2	G	70	PHE
2	G	74	GLU
2	G	80	CYS
3	H	5	LEU
4	I	5	THR
4	I	17	ARG
4	I	26	SER
4	I	66	ASN
4	I	81	LEU
4	I	84	THR
4	I	120	LYS
4	I	124	ILE
4	I	126	ILE
4	I	172	CYS
4	I	174	LEU
4	I	193	SER
5	J	55	TYR
5	J	59	GLU
5	J	70	ARG
5	J	92	GLN
5	J	94	THR
5	J	111	ASP

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Mol	Chain	Res	Type
5	J	125	THR
5	J	188	GLN
5	J	237	THR
1	K	88	SER
1	K	103	VAL
1	K	110	LEU
1	K	178	THR
1	K	197	HIS
1	K	230	LEU
1	K	232	GLU
1	K	239	ARG
1	K	261	VAL
2	L	2	GLN
2	L	4	THR
2	L	58	LYS
2	L	70	PHE
2	L	74	GLU
2	L	80	CYS
3	M	4	LEU
3	M	5	LEU
4	N	5	THR
4	N	17	ARG
4	N	26	SER
4	N	57	LEU
4	N	66	ASN
4	N	81	LEU
4	N	84	THR
4	N	120	LYS
4	N	124	ILE
4	N	126	ILE
4	N	172	CYS
4	N	174	LEU
4	N	193	SER
5	O	55	TYR
5	O	59	GLU
5	O	70	ARG
5	O	92	GLN
5	O	94	THR
5	O	111	ASP
5	O	125	THR
5	O	188	GLN
5	O	237	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	77	ASN
1	A	96	GLN
1	A	144	GLN
1	A	155	GLN
1	A	188	HIS
3	C	3	ASN
4	D	20	ASN
4	D	44	GLN
4	D	135	GLN
5	E	61	GLN
5	E	92	GLN
5	E	220	HIS
5	E	238	GLN
1	F	70	ASN
1	F	77	ASN
1	F	96	GLN
1	F	144	GLN
1	F	188	HIS
1	F	263	HIS
4	I	20	ASN
4	I	44	GLN
5	J	61	GLN
5	J	92	GLN
5	J	220	HIS
5	J	238	GLN
1	K	70	ASN
1	K	77	ASN
1	K	96	GLN
1	K	144	GLN
1	K	188	HIS
1	K	263	HIS
4	N	20	ASN
4	N	44	GLN
4	N	135	GLN
5	O	61	GLN
5	O	92	GLN
5	O	167	HIS
5	O	238	GLN

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 monosaccharides 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	276/276 (100%)	-0.13	1 (0%) 92 90	64, 64, 64, 64	13 (4%)
1	F	276/276 (100%)	-0.16	0 100 100	64, 64, 64, 64	12 (4%)
1	K	276/276 (100%)	0.14	14 (5%) 28 25	64, 64, 64, 64	16 (5%)
2	B	99/99 (100%)	0.05	0 100 100	64, 64, 64, 64	6 (6%)
2	G	99/99 (100%)	-0.11	0 100 100	64, 64, 64, 64	5 (5%)
2	L	99/99 (100%)	0.31	3 (3%) 50 44	64, 64, 64, 64	9 (9%)
3	C	10/10 (100%)	-0.09	0 100 100	64, 64, 64, 64	0
3	H	10/10 (100%)	0.08	0 100 100	64, 64, 64, 64	3 (30%)
3	M	10/10 (100%)	-0.13	0 100 100	64, 64, 64, 64	0
4	D	199/199 (100%)	-0.22	0 100 100	64, 64, 64, 65	13 (6%)
4	I	199/199 (100%)	0.03	4 (2%) 65 60	64, 64, 64, 65	17 (8%)
4	N	199/199 (100%)	0.12	5 (2%) 57 51	64, 64, 64, 65	21 (10%)
5	E	244/244 (100%)	-0.25	1 (0%) 92 90	25, 64, 64, 65	21 (8%)
5	J	244/244 (100%)	-0.21	1 (0%) 92 90	25, 64, 64, 65	20 (8%)
5	O	244/244 (100%)	-0.02	2 (0%) 86 81	25, 64, 64, 65	20 (8%)
All	All	2484/2484 (100%)	-0.06	31 (1%) 79 73	25, 64, 64, 65	176 (7%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	O	209	VAL	4.2
1	K	228	THR	3.9
5	E	2	THR	3.8
1	K	201	LEU	3.7
4	I	215	PRO	3.7
2	L	20	SER	3.1
5	J	2	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	193	PRO	2.9
1	K	200	THR	2.8
1	K	247	VAL	2.7
1	K	1	GLY	2.7
1	K	276	PRO	2.6
1	K	199	VAL	2.6
4	N	216	GLU	2.6
2	L	98	ASP	2.5
1	K	249	VAL	2.5
4	I	91	LEU	2.5
1	K	218	GLN	2.4
4	N	142	SER	2.3
4	I	216	GLU	2.3
1	K	195	SER	2.3
2	L	1	ILE	2.3
1	K	258	THR	2.2
4	I	142	SER	2.2
1	K	196	ASP	2.2
1	K	229	GLU	2.1
5	O	251	GLU	2.1
1	A	247	VAL	2.1
4	N	200	ALA	2.0
4	N	208	GLU	2.0
4	N	141	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.