



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:44 AM GMT

PDB ID : 2NX5
Title : Crystal structure of ELS4 TCR bound to HLA-B*3501 presenting EBV peptide EPLPQGQLTAY at 1.7Å
Authors : Tynan, F.E.; Reid, H.H.; Rossjohn, J.
Deposited on : 2006-11-16
Resolution : 2.70 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

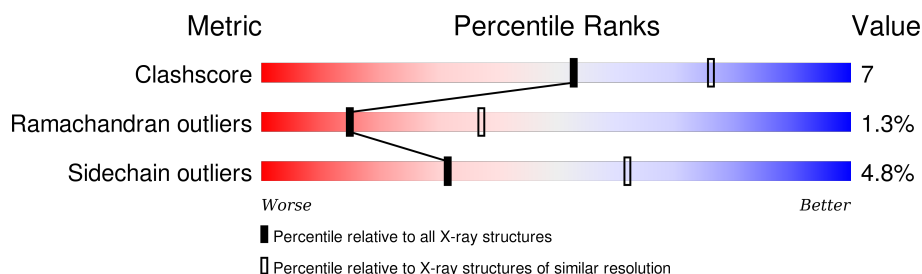
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)





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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	276	
1	F	276	
1	K	276	
1	Q	276	
2	B	99	
2	G	99	
2	L	99	

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Mol	Chain	Length	Quality of chain
2	R	99	 80% 20%
3	C	11	 55% 45%
3	H	11	 45% 27% 27%
3	M	11	 45% 36% 18%
3	S	11	 36% 55% 9%
4	D	188	 77% 20% •
4	I	188	 76% 21% ••
4	N	188	 76% 22% •
4	T	188	 76% 23% •
5	E	243	 81% 16% •
5	J	243	 84% 16% •
5	P	243	 82% 15% •
5	U	243	 81% 17% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26481 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-B35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1405	411	431	7			
1	F	276	Total	C	N	O	S	0	0	0
			2254	1405	411	431	7			
1	K	276	Total	C	N	O	S	0	0	0
			2254	1405	411	431	7			
1	Q	276	Total	C	N	O	S	0	0	0
			2254	1405	411	431	7			

- 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	0	0
			829	528	140	158	3			
2	L	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	R	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called EBV peptide, EPLPQGQLTAY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			86	55	13	18			
3	H	11	Total	C	N	O	0	0	0
			86	55	13	18			
3	M	11	Total	C	N	O	0	0	0
			86	55	13	18			
3	S	11	Total	C	N	O	0	0	0
			86	55	13	18			

- Molecule 4 is a protein called ELS4 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	188	Total	C	N	O	S	0	0	0
			1466	919	241	297	9			
4	I	188	Total	C	N	O	S	0	0	0
			1467	920	241	297	9			
4	N	188	Total	C	N	O	S	0	0	0
			1467	920	241	297	9			
4	T	188	Total	C	N	O	S	0	0	0
			1467	920	241	297	9			

- Molecule 5 is a protein called ELS4 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1936	1208	342	380	6			
5	J	243	Total	C	N	O	S	0	0	0
			1936	1208	342	380	6			
5	P	243	Total	C	N	O	S	0	0	0
			1936	1208	342	380	6			
5	U	243	Total	C	N	O	S	0	0	0
			1936	1208	342	380	6			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total	O	0	0
			17	17		
6	B	4	Total	O	0	0
			4	4		
6	C	1	Total	O	0	0
			1	1		
6	D	18	Total	O	0	0
			18	18		
6	E	5	Total	O	0	0
			5	5		
6	F	18	Total	O	0	0
			18	18		
6	G	4	Total	O	0	0
			4	4		
6	I	21	Total	O	0	0
			21	21		
6	J	10	Total	O	0	0
			10	10		

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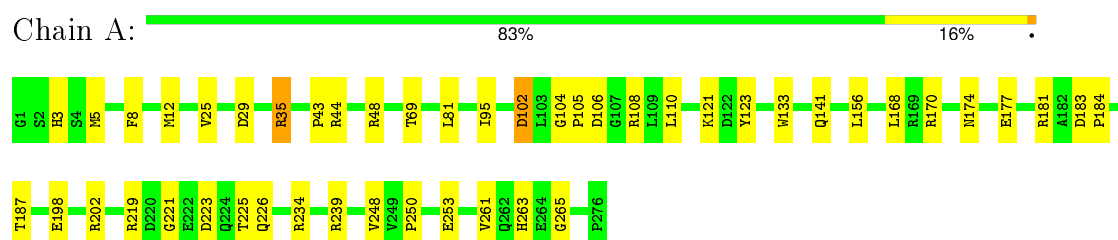
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	14	Total 14	O 14	0	0
6	L	6	Total 6	O 6	0	0
6	N	16	Total 16	O 16	0	0
6	P	20	Total 20	O 20	0	0
6	Q	15	Total 15	O 15	0	0
6	R	5	Total 5	O 5	0	0
6	T	10	Total 10	O 10	0	0
6	U	10	Total 10	O 10	0	0

3 Residue-property plots [i](#)

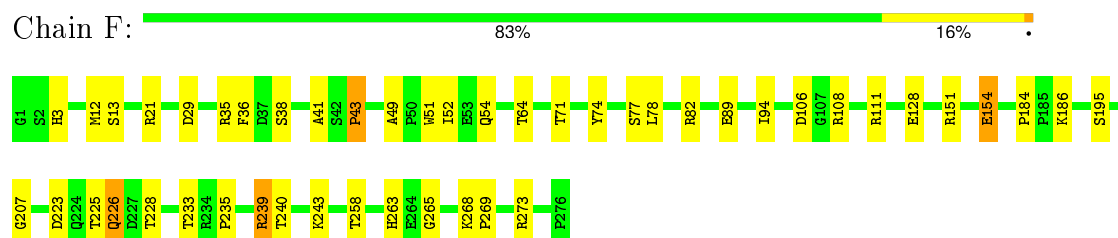
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

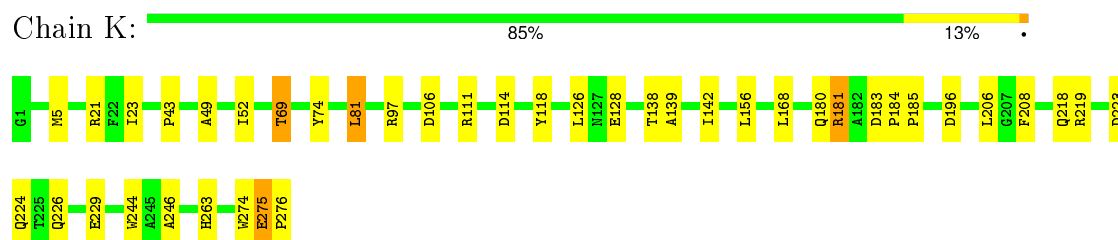
• Molecule 1: HLA-B35



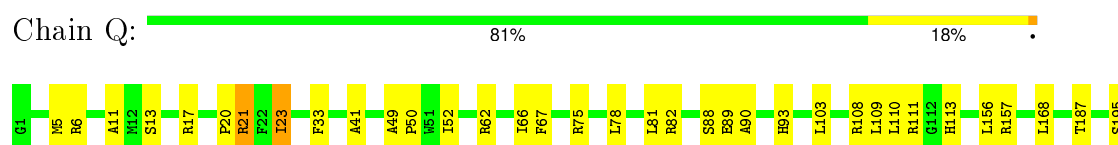
• Molecule 1: HLA-B35



• Molecule 1: HLA-B35



• Molecule 1: HLA-B35

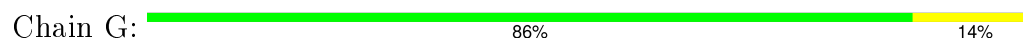




• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



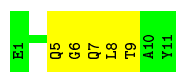
• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



• Molecule 3: EBV peptide, EPLPQGQLTAY



• Molecule 3: EBV peptide, EPLPQGQLTAY

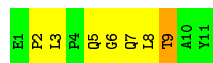


• Molecule 3: EBV peptide, EPLPQGQLTAY




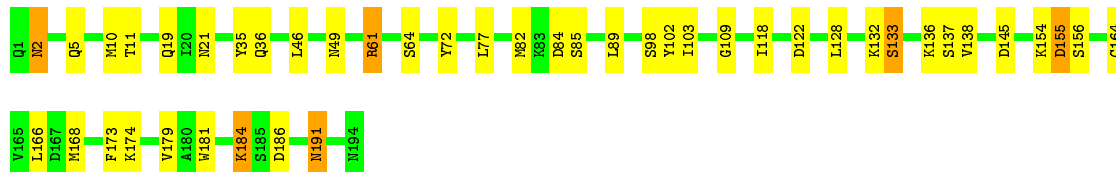
- Molecule 3: EBV peptide, EPLPQGQLTAY

Chain S: 



- Molecule 4: ELS4 TCR alpha chain

Chain D: 



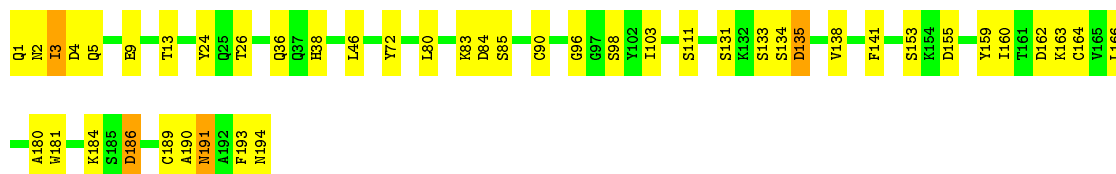
- Molecule 4: ELS4 TCR alpha chain

Chain I: 




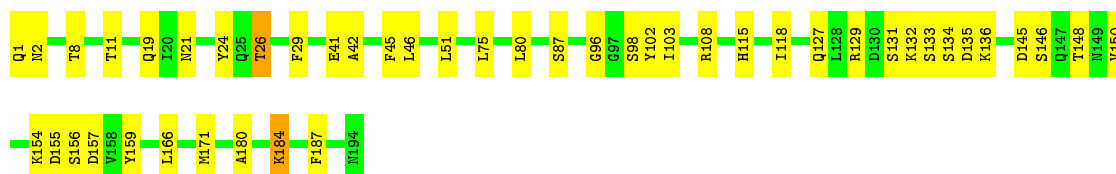
- Molecule 4: ELS4 TCR alpha chain

Chain N: 




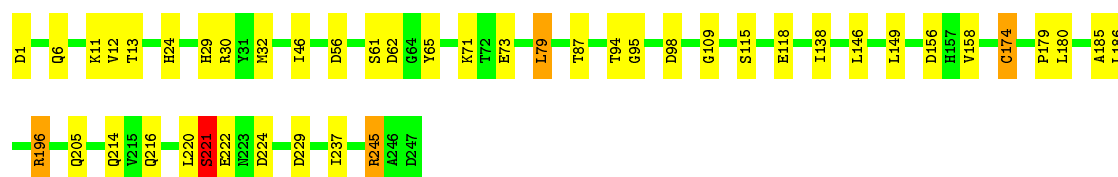
- Molecule 4: ELS4 TCR alpha chain

Chain T: 



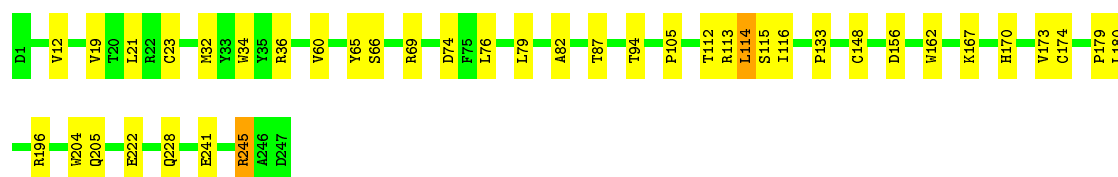
- Molecule 5: ELS4 TCR beta chain

Chain E: 



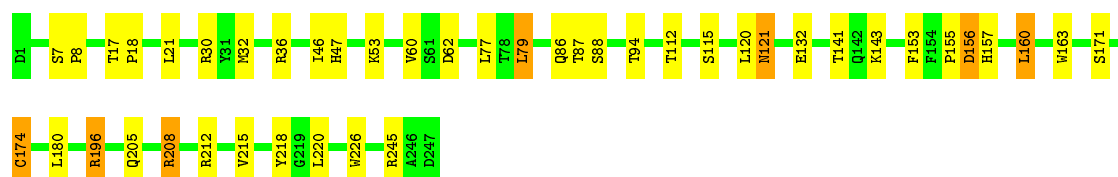
- Molecule 5: ELS4 TCR beta chain

Chain J: 84% 16% •



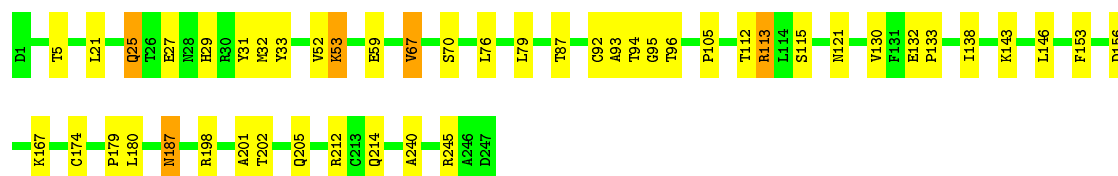
- Molecule 5: ELS4 TCR beta chain

Chain P: 82% 15% •



- Molecule 5: ELS4 TCR beta chain

Chain U: 81% 17% •



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.48Å 118.07Å 131.47Å 90.00° 96.04° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	93.5 (30.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.269 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26481	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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	0.33	0/2317	0.52	0/3150
1	F	0.33	0/2317	0.50	0/3150
1	K	0.33	0/2317	0.50	0/3150
1	Q	0.34	0/2317	0.51	0/3150
2	B	0.34	0/852	0.45	0/1152
2	G	0.34	0/852	0.47	0/1152
2	L	0.35	0/852	0.48	0/1152
2	R	0.35	0/852	0.47	0/1152
3	C	0.43	0/88	0.60	0/119
3	H	0.44	0/88	0.70	0/119
3	M	0.37	0/88	0.56	0/119
3	S	0.38	0/88	0.52	0/119
4	D	0.35	0/1498	0.58	0/2027
4	I	0.36	0/1499	0.54	0/2028
4	N	0.36	0/1499	0.55	0/2028
4	T	0.37	0/1499	0.55	0/2028
5	E	0.35	0/1989	0.50	0/2707
5	J	0.33	0/1989	0.50	0/2707
5	P	0.35	0/1989	0.52	0/2707
5	U	0.35	0/1989	0.49	0/2707
All	All	0.34	0/26979	0.51	0/36623

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
4	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	136	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2254	0	2117	23	0
1	F	2254	0	2117	28	0
1	K	2254	0	2117	24	0
1	Q	2254	0	2117	32	0
2	B	829	0	794	4	0
2	G	829	0	794	6	0
2	L	829	0	794	7	0
2	R	829	0	794	14	0
3	C	86	0	84	5	0
3	H	86	0	84	7	0
3	M	86	0	84	5	0
3	S	86	0	84	6	0
4	D	1466	0	1382	26	0
4	I	1467	0	1387	26	0
4	N	1467	0	1387	23	0
4	T	1467	0	1387	36	0
5	E	1936	0	1817	25	0
5	J	1936	0	1817	21	0
5	P	1936	0	1817	33	0
5	U	1936	0	1817	29	0
6	A	17	0	0	0	0
6	B	4	0	0	1	0
6	C	1	0	0	0	0
6	D	18	0	0	0	0
6	E	5	0	0	0	0
6	F	18	0	0	0	0
6	G	4	0	0	0	0
6	I	21	0	0	0	0
6	J	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	14	0	0	0	0
6	L	6	0	0	1	0
6	N	16	0	0	0	0
6	P	20	0	0	1	0
6	Q	15	0	0	0	0
6	R	5	0	0	0	0
6	T	10	0	0	0	0
6	U	10	0	0	0	0
All	All	26481	0	24791	335	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 7.

All (335) 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)
3:H:5:GLN:HB2	3:H:9:THR:HG21	1.17	1.13
5:P:208:ARG:HH11	5:P:208:ARG:HG3	1.16	1.07
4:T:129:ARG:HG2	4:T:129:ARG:HH21	1.27	0.97
1:Q:20:PRO:HB2	1:Q:75:ARG:HG2	1.47	0.96
1:Q:20:PRO:HB3	1:Q:78:LEU:HD13	1.49	0.95
4:T:108:ARG:HG2	4:T:108:ARG:HH11	1.32	0.95
3:S:5:GLN:HB3	3:S:9:THR:HG21	1.50	0.91
4:D:138:VAL:HG23	4:D:181:TRP:HB3	1.58	0.84
2:R:23:LEU:HD23	2:R:39:LEU:HD21	1.60	0.83
3:C:5:GLN:HB2	3:C:9:THR:HG21	1.62	0.81
4:T:19:GLN:HE21	4:T:21:ASN:HD21	1.28	0.80
3:C:6:GLY:O	3:C:9:THR:HG22	1.83	0.79
4:D:164:CYS:HB3	5:E:196:ARG:HH22	1.47	0.78
1:F:263:HIS:CD2	1:F:265:GLY:H	2.03	0.77
4:T:131:SER:HB2	5:U:132:GLU:CG	2.18	0.73
5:P:87:THR:HG23	5:P:115:SER:HA	1.71	0.73
5:J:156:ASP:HB2	5:J:179:PRO:HG3	1.69	0.72
4:T:26:THR:HG23	4:T:29:PHE:HB2	1.69	0.72
5:P:208:ARG:NH1	5:P:208:ARG:HG3	1.94	0.72
1:K:21:ARG:HE	1:K:23:ILE:HD11	1.53	0.71
1:Q:13:SER:HB2	1:Q:78:LEU:HD22	1.72	0.71
4:I:32:LEU:HD12	4:I:92:VAL:HG22	1.72	0.71
4:T:24:TYR:CD1	4:T:26:THR:HG22	2.26	0.70
1:F:239:ARG:HD3	1:F:239:ARG:O	1.92	0.69
1:K:111:ARG:HH12	1:K:128:GLU:HG3	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:98:SER:O	4:I:103:ILE:N	2.23	0.68
4:T:129:ARG:HG2	4:T:129:ARG:NH2	2.04	0.68
4:T:166:LEU:HB3	5:U:174:CYS:HB2	1.76	0.68
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.74	0.68
4:I:24:TYR:HD1	4:I:26:THR:HG22	1.58	0.68
5:E:220:LEU:O	5:E:221:SER:HB2	1.93	0.67
4:D:155:ASP:H	1:F:184:PRO:HD2	1.58	0.67
4:D:166:LEU:HB3	5:E:174:CYS:HB3	1.76	0.66
2:L:70:PHE:CE2	2:L:72:PRO:HG3	2.30	0.66
3:H:6:GLY:HA2	5:P:30:ARG:HH22	1.62	0.65
4:I:24:TYR:CD1	4:I:26:THR:HG22	2.31	0.65
4:T:131:SER:HB2	5:U:132:GLU:HG3	1.78	0.65
1:K:69:THR:HG23	5:P:30:ARG:NH2	2.13	0.64
4:I:132:LYS:HD3	5:J:241:GLU:H	1.62	0.64
4:T:132:LYS:HG2	5:U:240:ALA:HB1	1.80	0.64
2:B:2:GLN:HG2	2:B:86:THR:HG22	1.80	0.63
1:A:177:GLU:HG2	1:A:181:ARG:HH12	1.64	0.63
1:F:233:THR:OG1	1:F:243:LYS:NZ	2.32	0.63
4:D:179:VAL:CG2	5:E:196:ARG:HE	2.11	0.63
1:F:82:ARG:HD3	1:F:89:GLU:HG2	1.80	0.63
5:J:82:ALA:HB1	5:J:116:ILE:HD13	1.80	0.62
4:T:24:TYR:HD1	4:T:26:THR:HG22	1.64	0.61
2:G:36:GLU:O	2:G:82:VAL:HA	2.00	0.61
1:A:263:HIS:CD2	1:A:265:GLY:H	2.17	0.61
3:S:7:GLN:O	3:S:8:LEU:HB2	2.01	0.61
4:T:108:ARG:HG2	4:T:108:ARG:NH1	2.11	0.61
1:Q:62:ARG:O	1:Q:66:ILE:HG12	2.01	0.60
4:D:82:MET:HG3	4:D:174:LYS:HE2	1.82	0.60
1:F:12:MET:HG2	1:F:94:ILE:HG12	1.83	0.60
3:C:7:GLN:O	3:C:8:LEU:HB2	2.01	0.60
1:A:104:GLY:C	1:A:106:ASP:H	2.05	0.59
1:F:258:THR:HG22	1:F:273:ARG:HG2	1.83	0.59
1:F:151:ARG:HH21	1:F:154:GLU:HG2	1.66	0.59
1:Q:88:SER:C	1:Q:90:ALA:H	2.06	0.59
4:T:108:ARG:HH11	4:T:108:ARG:CG	2.12	0.58
5:J:170:HIS:O	5:J:173:VAL:HB	2.04	0.58
4:N:24:TYR:HD1	4:N:26:THR:HG22	1.68	0.57
1:F:263:HIS:HD2	1:F:265:GLY:H	1.52	0.57
4:I:132:LYS:HD2	5:J:241:GLU:HG2	1.85	0.57
4:D:184:LYS:HE3	4:D:186:ASP:O	2.04	0.57
2:R:84:HIS:H	2:R:87:LEU:HD12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:53:LYS:HA	5:P:53:LYS:HE2	1.86	0.57
3:S:7:GLN:HB2	5:U:96:THR:HB	1.85	0.57
4:D:128:LEU:O	4:D:137:SER:HB2	2.04	0.57
5:P:121:ASN:HA	5:P:226:TRP:HZ3	1.70	0.57
2:L:1:ILE:HG12	2:L:2:GLN:HG3	1.87	0.57
5:E:220:LEU:O	5:E:221:SER:CB	2.53	0.57
4:D:154:LYS:C	4:D:156:SER:H	2.08	0.57
1:K:244:TRP:HZ3	1:K:246:ALA:HB2	1.68	0.57
5:P:163:TRP:HB2	5:P:212:ARG:HB3	1.86	0.57
4:N:24:TYR:CD1	4:N:26:THR:HG22	2.40	0.56
5:P:46:ILE:HD13	5:P:60:VAL:HG23	1.87	0.56
1:Q:13:SER:HB3	1:Q:93:HIS:H	1.70	0.56
1:K:114:ASP:OD2	1:K:156:LEU:HD21	2.05	0.56
4:N:5:GLN:HE22	4:N:90:CYS:H	1.52	0.56
1:K:218:GLN:HA	1:K:223:ASP:HA	1.86	0.56
1:F:49:ALA:O	1:F:52:ILE:HG22	2.06	0.56
4:T:159:TYR:O	4:T:180:ALA:HA	2.06	0.56
3:H:7:GLN:O	3:H:9:THR:N	2.39	0.55
2:L:72:PRO:HD2	6:L:103:HOH:O	2.07	0.55
1:Q:33:PHE:HD2	1:Q:52:ILE:HD13	1.71	0.55
5:J:205:GLN:HA	5:J:245:ARG:O	2.07	0.55
5:E:174:CYS:SG	5:E:196:ARG:NH2	2.80	0.55
4:N:153:SER:HB3	4:N:160:ILE:H	1.72	0.54
4:T:129:ARG:HH21	4:T:129:ARG:CG	2.11	0.54
4:D:98:SER:O	4:D:103:ILE:N	2.37	0.54
1:K:69:THR:HG23	5:P:30:ARG:HH21	1.73	0.54
4:D:179:VAL:HG23	5:E:196:ARG:HE	1.73	0.54
4:D:21:ASN:ND2	4:D:72:TYR:OH	2.41	0.54
4:T:41:GLU:HG2	4:T:42:ALA:H	1.72	0.53
4:T:45:PHE:CD1	5:U:105:PRO:HB3	2.43	0.53
4:D:11:THR:O	1:Q:108:ARG:NH1	2.37	0.53
1:Q:210:PRO:O	1:Q:263:HIS:HE1	1.90	0.53
5:P:208:ARG:CG	5:P:208:ARG:HH11	2.05	0.53
4:T:131:SER:HB2	5:U:132:GLU:HG2	1.89	0.53
4:D:98:SER:C	4:D:103:ILE:H	2.11	0.53
5:E:71:LYS:HD2	5:E:73:GLU:HB2	1.90	0.53
1:F:13:SER:HB3	1:F:78:LEU:HD22	1.91	0.53
5:J:114:LEU:HD21	5:J:116:ILE:HD11	1.90	0.53
1:Q:235:PRO:HG2	2:R:65:LEU:HD13	1.91	0.53
5:P:32:MET:HG2	5:P:94:THR:HG22	1.91	0.52
3:H:11:TYR:HB3	1:K:81:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLU:HG2	1:A:248:VAL:HG12	1.91	0.52
5:P:174:CYS:SG	5:P:196:ARG:HD3	2.50	0.52
3:H:7:GLN:C	3:H:9:THR:H	2.12	0.52
1:A:170:ARG:HE	1:A:174:ASN:HD21	1.58	0.52
1:F:207:GLY:HA2	1:F:240:THR:HB	1.90	0.52
4:I:166:LEU:HB3	5:J:174:CYS:HB2	1.92	0.52
3:H:6:GLY:O	3:H:9:THR:HG22	2.10	0.52
4:N:134:SER:O	4:N:135:ASP:HB2	2.10	0.52
5:E:24:HIS:CD2	5:E:73:GLU:HB3	2.45	0.52
4:N:38:HIS:HE1	4:N:83:LYS:O	1.93	0.52
1:Q:5:MET:HB2	1:Q:168:LEU:HD13	1.91	0.51
4:N:141:PHE:HB2	4:N:193:PHE:CZ	2.46	0.51
4:I:98:SER:C	4:I:103:ILE:H	2.11	0.51
5:E:87:THR:HG23	5:E:115:SER:HA	1.92	0.51
5:P:79:LEU:N	5:P:79:LEU:HD23	2.25	0.51
1:A:184:PRO:HD2	4:I:155:ASP:H	1.74	0.51
5:J:69:ARG:HD2	5:J:74:ASP:O	2.11	0.51
2:R:39:LEU:HD22	2:R:46:ILE:HG13	1.91	0.51
4:N:9:GLU:HG3	4:N:111:SER:HB2	1.93	0.51
4:D:191:ASN:C	4:D:191:ASN:HD22	2.14	0.51
5:E:185:ALA:HB1	1:F:239:ARG:HH11	1.75	0.51
5:U:21:LEU:HD21	5:U:112:THR:HG21	1.93	0.50
1:F:3:HIS:HD2	1:F:29:ASP:OD2	1.95	0.50
5:E:12:VAL:HG12	5:E:115:SER:HB3	1.93	0.50
5:J:32:MET:HG2	5:J:94:THR:HG22	1.92	0.50
4:T:26:THR:CG2	4:T:29:PHE:HB2	2.38	0.50
5:U:53:LYS:HE2	5:U:70:SER:HA	1.92	0.50
2:R:46:ILE:HG21	2:R:68:THR:HG21	1.92	0.50
1:F:111:ARG:CZ	1:F:128:GLU:HG3	2.42	0.50
1:Q:229:GLU:HB3	1:Q:246:ALA:HB3	1.94	0.50
4:T:127:GLN:HE21	4:T:129:ARG:HH22	1.60	0.50
1:Q:23:ILE:HD13	2:R:54:LEU:HD23	1.93	0.50
4:D:49:ASN:OD1	4:D:64:SER:HB3	2.11	0.50
1:F:235:PRO:HG2	2:G:65:LEU:HD13	1.93	0.49
1:Q:263:HIS:CD2	1:Q:265:GLY:H	2.30	0.49
4:T:98:SER:C	4:T:103:ILE:H	2.15	0.49
1:Q:187:THR:HG21	1:Q:261:VAL:HG21	1.94	0.49
1:Q:11:ALA:HA	1:Q:21:ARG:O	2.13	0.49
1:Q:111:ARG:HE	1:Q:113:HIS:CE1	2.30	0.49
1:F:21:ARG:HG3	1:F:38:SER:OG	2.12	0.49
1:Q:206:LEU:HD23	1:Q:242:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:131:SER:HB2	5:P:132:GLU:HG3	1.93	0.49
3:M:7:GLN:C	3:M:9:THR:H	2.15	0.49
2:R:21:ASN:HB3	2:R:70:PHE:CE1	2.47	0.49
4:I:184:LYS:HG2	4:I:186:ASP:H	1.76	0.49
4:I:38:HIS:HE1	4:I:83:LYS:O	1.96	0.49
4:D:168:MET:HB2	4:D:173:PHE:HB3	1.95	0.48
5:P:21:LEU:HD12	5:P:77:LEU:HD23	1.95	0.48
2:R:51:HIS:HD2	2:R:64:LEU:HD22	1.77	0.48
1:F:77:SER:HB3	3:M:11:TYR:HB2	1.95	0.48
4:T:24:TYR:CE1	4:T:26:THR:HG22	2.48	0.48
5:P:141:THR:HB	5:P:143:LYS:HD2	1.95	0.48
5:P:208:ARG:CG	5:P:208:ARG:NH1	2.71	0.48
5:P:153:PHE:HE1	5:P:156:ASP:HA	1.78	0.48
5:P:46:ILE:HG22	5:P:47:HIS:CD2	2.49	0.48
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.96	0.48
1:K:229:GLU:N	1:K:246:ALA:O	2.43	0.47
1:F:51:TRP:O	1:F:54:GLN:HG2	2.14	0.47
1:F:41:ALA:O	1:F:43:PRO:HD3	2.14	0.47
5:P:157:HIS:HB3	5:P:218:TYR:HB2	1.95	0.47
1:A:8:PHE:HB2	1:A:25:VAL:HG23	1.95	0.47
1:Q:20:PRO:HB3	1:Q:78:LEU:CD1	2.33	0.47
5:P:46:ILE:HG22	5:P:47:HIS:HD2	1.78	0.47
4:N:184:LYS:HE3	4:N:186:ASP:HB2	1.96	0.47
1:Q:33:PHE:CD2	1:Q:52:ILE:HD13	2.49	0.47
4:I:38:HIS:HB2	4:I:41:GLU:HG2	1.96	0.47
2:B:13:HIS:H	2:B:21:ASN:HD21	1.62	0.47
4:I:138:VAL:HG22	4:I:181:TRP:HB3	1.97	0.47
1:A:133:TRP:HH2	1:A:156:LEU:CD1	2.28	0.47
4:I:18:VAL:HG12	4:I:77:LEU:HB2	1.97	0.47
2:G:59:ASP:O	2:G:60:TRP:HB2	2.15	0.47
4:T:108:ARG:NH1	4:T:108:ARG:CG	2.76	0.46
1:K:81:LEU:HD12	1:K:118:TYR:CD1	2.51	0.46
4:N:189:CYS:O	4:N:191:ASN:N	2.48	0.46
4:N:166:LEU:HB3	5:P:174:CYS:HB3	1.97	0.46
4:D:118:ILE:HG13	4:D:145:ASP:HA	1.97	0.46
4:I:134:SER:O	4:I:135:ASP:HB2	2.15	0.46
1:K:5:MET:HB2	1:K:168:LEU:HD13	1.97	0.46
1:K:126:LEU:HD22	1:K:156:LEU:HD23	1.97	0.46
2:R:51:HIS:HA	2:R:65:LEU:O	2.15	0.46
5:U:32:MET:HG2	5:U:94:THR:HG22	1.95	0.46
2:G:17:ASN:HD21	2:G:74:GLU:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:21:ASN:OD1	2:G:22:PHE:N	2.44	0.46
5:J:174:CYS:SG	5:J:196:ARG:HD2	2.56	0.46
5:P:120:LEU:HD22	5:P:220:LEU:HD21	1.96	0.46
5:J:23:CYS:HB2	5:J:34:TRP:CZ2	2.51	0.46
4:I:70:LYS:HE2	4:N:72:TYR:CG	2.50	0.46
5:U:87:THR:HG23	5:U:115:SER:HA	1.97	0.46
4:N:138:VAL:HG22	4:N:181:TRP:HB3	1.97	0.46
4:N:153:SER:HB3	4:N:160:ILE:N	2.30	0.46
4:N:159:TYR:O	4:N:180:ALA:HA	2.16	0.46
2:L:12:ARG:HE	2:L:22:PHE:HB2	1.81	0.46
4:D:5:GLN:NE2	4:D:109:GLY:H	2.14	0.46
1:Q:268:LYS:HG3	1:Q:269:PRO:HD2	1.97	0.46
1:F:223:ASP:HB3	1:F:225:THR:HG23	1.98	0.46
4:D:36:GLN:HB2	4:D:46:LEU:HD11	1.98	0.46
1:A:81:LEU:HD21	1:A:123:TYR:CZ	2.51	0.46
1:K:275:GLU:HA	1:K:276:PRO:HD3	1.81	0.45
5:P:21:LEU:HD22	5:P:112:THR:HG21	1.98	0.45
1:Q:203:CYS:HB2	1:Q:217:TRP:CZ2	2.50	0.45
1:K:208:PHE:CD2	1:K:263:HIS:HE1	2.34	0.45
5:J:87:THR:HG23	5:J:115:SER:HA	1.99	0.45
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.99	0.45
5:P:121:ASN:HA	5:P:226:TRP:CZ3	2.52	0.45
4:T:133:SER:O	4:T:134:SER:HB3	2.17	0.45
4:T:24:TYR:CD1	4:T:26:THR:CG2	2.98	0.45
5:P:36:ARG:HH12	5:P:86:GLN:HA	1.81	0.45
1:A:223:ASP:HB3	1:A:225:THR:HG23	1.99	0.45
1:K:49:ALA:O	1:K:52:ILE:HG22	2.16	0.45
1:F:106:ASP:OD1	4:N:13:THR:HB	2.17	0.45
4:I:62:PHE:CD1	4:I:77:LEU:HD22	2.51	0.45
3:H:6:GLY:HA2	5:P:30:ARG:NH2	2.30	0.45
5:E:221:SER:OG	5:E:222:GLU:HA	2.17	0.45
5:P:205:GLN:HA	5:P:245:ARG:O	2.17	0.45
2:L:70:PHE:HD2	2:L:78:TYR:CZ	2.35	0.44
4:D:35:TYR:HB2	4:D:89:LEU:HB2	1.99	0.44
4:N:80:LEU:HD12	4:N:84:ASP:OD2	2.17	0.44
4:I:23:THR:HG22	4:I:72:TYR:HD1	1.82	0.44
3:S:6:GLY:O	3:S:9:THR:HG22	2.17	0.44
1:F:106:ASP:OD2	1:F:108:ARG:N	2.36	0.44
5:J:19:VAL:HG11	5:J:114:LEU:HD11	2.00	0.44
5:U:31:TYR:O	5:U:94:THR:HA	2.17	0.44
4:T:154:LYS:C	4:T:156:SER:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:132:LYS:HG2	5:U:240:ALA:CB	2.47	0.43
1:F:74:TYR:CE2	3:M:11:TYR:HE1	2.35	0.43
5:J:133:PRO:HD2	5:J:204:TRP:CZ2	2.53	0.43
1:Q:67:PHE:CZ	3:S:2:PRO:HB3	2.53	0.43
3:M:3:LEU:HD23	3:M:5:GLN:CG	2.48	0.43
5:U:25:GLN:HG2	5:U:27:GLU:H	1.82	0.43
1:A:250:PRO:O	1:A:253:GLU:HB2	2.18	0.43
2:G:71:THR:HA	2:G:72:PRO:HD3	1.86	0.43
4:T:115:HIS:CG	4:T:146:SER:HB3	2.52	0.43
5:U:133:PRO:HG3	5:U:146:LEU:HD12	2.00	0.43
2:R:39:LEU:HD13	2:R:68:THR:HG22	2.00	0.43
1:K:274:TRP:CH2	1:K:276:PRO:HA	2.53	0.43
2:L:54:LEU:HD12	2:L:64:LEU:HD21	2.00	0.43
5:E:11:LYS:HD2	5:E:13:THR:HG23	2.00	0.43
4:D:82:MET:CG	4:D:174:LYS:HE2	2.48	0.43
5:J:69:ARG:O	5:J:69:ARG:HG3	2.17	0.43
4:I:5:GLN:HE22	4:I:90:CYS:H	1.65	0.43
1:A:202:ARG:HD2	6:B:100:HOH:O	2.19	0.43
1:K:244:TRP:CZ3	1:K:246:ALA:HB2	2.52	0.43
5:U:32:MET:HA	5:U:93:ALA:O	2.18	0.43
4:T:129:ARG:NH2	4:T:129:ARG:CG	2.74	0.43
5:U:156:ASP:HB2	5:U:179:PRO:HG2	2.00	0.43
4:I:46:LEU:HD22	4:I:62:PHE:HD2	1.84	0.43
1:F:226:GLN:C	1:F:228:THR:H	2.21	0.43
5:J:21:LEU:HD22	5:J:112:THR:HG21	2.00	0.43
3:S:8:LEU:HD23	5:U:96:THR:HG21	2.01	0.43
1:F:36:PHE:HE2	1:F:64:THR:HG23	1.84	0.43
5:U:33:TYR:O	5:U:92:CYS:HA	2.19	0.43
1:Q:6:ARG:HH12	1:Q:113:HIS:HB2	1.84	0.43
4:I:186:ASP:OD2	4:I:186:ASP:N	2.52	0.43
5:E:29:HIS:HB3	5:E:95:GLY:O	2.19	0.43
1:K:184:PRO:HA	1:K:185:PRO:HD3	1.93	0.43
5:J:21:LEU:HD21	5:J:114:LEU:HD13	2.01	0.42
5:P:160:LEU:HG	5:P:215:VAL:HG22	2.00	0.42
4:I:45:PHE:CD1	5:J:105:PRO:HB3	2.54	0.42
1:F:268:LYS:HD2	1:F:269:PRO:HD2	2.01	0.42
2:B:21:ASN:CG	2:B:22:PHE:H	2.22	0.42
5:E:205:GLN:HA	5:E:245:ARG:O	2.18	0.42
3:C:6:GLY:HA2	5:E:30:ARG:NH2	2.35	0.42
5:E:156:ASP:HB2	5:E:179:PRO:HG2	2.01	0.42
5:E:46:ILE:O	5:E:61:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:ASP:HB3	1:F:184:PRO:HG2	2.02	0.42
5:U:25:GLN:OE1	5:U:29:HIS:N	2.50	0.42
4:D:10:MET:HE1	4:D:19:GLN:O	2.19	0.42
5:U:138:ILE:HG23	5:U:201:ALA:HB1	2.01	0.42
1:Q:236:ALA:O	2:R:12:ARG:HG3	2.18	0.42
5:P:17:THR:HA	5:P:18:PRO:HD3	1.93	0.42
1:K:244:TRP:HZ3	1:K:246:ALA:CB	2.33	0.42
4:T:98:SER:O	4:T:103:ILE:N	2.50	0.42
1:A:81:LEU:HD12	1:A:95:ILE:HD11	2.02	0.42
1:A:234:ARG:HD2	2:B:10:TYR:CE1	2.55	0.42
1:K:74:TYR:OH	1:K:97:ARG:HD3	2.19	0.42
2:R:80:CYS:O	2:R:92:ILE:HA	2.20	0.42
1:A:219:ARG:C	1:A:221:GLY:H	2.23	0.42
1:Q:103:LEU:HD23	1:Q:109:LEU:HA	2.01	0.42
5:U:153:PHE:HE1	5:U:156:ASP:HA	1.85	0.42
1:K:219:ARG:HB2	1:K:224:GLN:HG3	2.02	0.42
4:N:3:ILE:HG12	4:N:3:ILE:H	1.58	0.42
4:D:61:ARG:HH22	4:D:84:ASP:CG	2.23	0.42
5:P:155:PRO:HG2	5:P:157:HIS:CD2	2.55	0.41
5:E:65:TYR:CD1	5:E:79:LEU:HD22	2.55	0.41
1:Q:214:THR:HB	1:Q:262:GLN:HB2	2.01	0.41
1:A:121:LYS:HB3	1:A:121:LYS:HE2	1.83	0.41
1:A:102:ASP:OD2	1:A:102:ASP:N	2.53	0.41
5:U:187:ASN:OD1	5:U:187:ASN:N	2.53	0.41
4:T:118:ILE:HG13	4:T:145:ASP:HA	2.01	0.41
1:Q:157:ARG:HG2	4:T:51:LEU:HD21	2.02	0.41
5:J:36:ARG:NH1	5:J:65:TYR:OH	2.53	0.41
5:U:130:VAL:HG23	5:U:240:ALA:HB3	2.03	0.41
3:C:7:GLN:O	5:E:98:ASP:OD2	2.37	0.41
2:R:5:PRO:HG3	2:R:84:HIS:HB2	2.02	0.41
5:E:32:MET:HG2	5:E:94:THR:HG22	2.01	0.41
1:K:139:ALA:HA	1:K:142:ILE:HD12	2.02	0.41
4:I:37:GLN:HB2	4:I:43:PRO:HB3	2.01	0.41
1:A:104:GLY:C	1:A:106:ASP:N	2.73	0.41
5:U:212:ARG:NH1	5:U:214:GLN:OE1	2.51	0.41
2:R:84:HIS:CE1	2:R:85:VAL:HG12	2.56	0.41
1:A:35:ARG:HG2	1:A:48:ARG:HD3	2.02	0.41
5:U:67:VAL:HA	5:U:76:LEU:O	2.20	0.41
3:M:7:GLN:O	3:M:9:THR:N	2.52	0.41
1:K:208:PHE:CD2	1:K:263:HIS:CE1	3.09	0.41
4:T:46:LEU:HD13	4:T:75:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:36:GLN:HB2	4:N:46:LEU:HD11	2.02	0.41
4:I:63:SER:HB2	4:I:76:LEU:HB3	2.03	0.41
4:I:76:LEU:HD23	4:I:78:LYS:HD2	2.01	0.41
4:T:171:MET:SD	5:U:143:LYS:HE3	2.61	0.41
4:T:184:LYS:O	4:T:187:PHE:HB2	2.21	0.41
5:E:214:GLN:HG3	5:E:237:ILE:CG2	2.51	0.41
1:Q:49:ALA:HA	1:Q:50:PRO:HD3	1.92	0.41
1:Q:6:ARG:HH12	1:Q:113:HIS:CG	2.39	0.41
5:U:31:TYR:HB2	5:U:95:GLY:O	2.21	0.41
1:A:108:ARG:NH1	4:T:11:THR:O	2.54	0.41
2:L:97:ARG:HD2	2:L:97:ARG:H	1.86	0.41
1:K:181:ARG:HH21	1:K:183:ASP:N	2.19	0.41
5:U:113:ARG:HH11	5:U:113:ARG:HB3	1.86	0.40
5:E:6:GLN:HE21	5:E:109:GLY:HA3	1.86	0.40
1:Q:6:ARG:HH22	1:Q:113:HIS:CD2	2.38	0.40
4:D:122:ASP:OD2	1:Q:269:PRO:HG2	2.22	0.40
4:N:164:CYS:HB2	6:P:248:HOH:O	2.21	0.40
5:E:158:VAL:HA	5:E:216:GLN:O	2.22	0.40
5:J:148:CYS:HB2	5:J:162:TRP:CZ2	2.56	0.40
4:N:98:SER:C	4:N:103:ILE:H	2.25	0.40
5:P:7:SER:HA	5:P:8:PRO:HA	1.89	0.40
4:N:162:ASP:OD1	4:N:163:LYS:N	2.53	0.40
4:I:61:ARG:NH1	4:I:79:GLU:O	2.54	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%)	263 (96%)	9 (3%)	2 (1%)	26 55
1	F	274/276 (99%)	254 (93%)	18 (7%)	2 (1%)	26 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	274/276 (99%)	258 (94%)	14 (5%)	2 (1%)	26	55
1	Q	274/276 (99%)	255 (93%)	15 (6%)	4 (2%)	13	32
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	G	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
2	L	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	19	45
2	R	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
3	C	9/11 (82%)	6 (67%)	3 (33%)	0	100	100
3	H	9/11 (82%)	6 (67%)	1 (11%)	2 (22%)	0	0
3	M	9/11 (82%)	6 (67%)	2 (22%)	1 (11%)	0	0
3	S	9/11 (82%)	7 (78%)	2 (22%)	0	100	100
4	D	186/188 (99%)	170 (91%)	12 (6%)	4 (2%)	8	22
4	I	186/188 (99%)	167 (90%)	13 (7%)	6 (3%)	5	12
4	N	186/188 (99%)	160 (86%)	19 (10%)	7 (4%)	4	9
4	T	186/188 (99%)	168 (90%)	13 (7%)	5 (3%)	6	16
5	E	241/243 (99%)	229 (95%)	10 (4%)	2 (1%)	24	51
5	J	241/243 (99%)	233 (97%)	8 (3%)	0	100	100
5	P	241/243 (99%)	227 (94%)	12 (5%)	2 (1%)	24	51
5	U	241/243 (99%)	227 (94%)	12 (5%)	2 (1%)	24	51
All	All	3228/3268 (99%)	3009 (93%)	177 (6%)	42 (1%)	15	37

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	102	TYR
4	N	135	ASP
4	N	191	ASN
4	T	135	ASP
4	D	2	ASN
4	D	133	SER
4	D	155	ASP
5	E	221	SER
5	E	224	ASP
3	H	7	GLN
3	H	8	LEU
4	I	136	LYS
4	N	2	ASN

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Mol	Chain	Res	Type
4	N	96	GLY
4	N	133	SER
4	N	155	ASP
4	N	190	ALA
1	Q	41	ALA
1	Q	195	SER
4	T	2	ASN
4	T	155	ASP
4	D	102	TYR
1	F	195	SER
3	M	8	LEU
1	Q	89	GLU
4	T	102	TYR
5	U	205	GLN
4	I	2	ASN
4	I	96	GLY
1	A	43	PRO
1	F	43	PRO
4	I	155	ASP
1	K	43	PRO
1	K	226	GLN
5	P	88	SER
5	P	156	ASP
1	Q	267	PRO
2	L	14	PRO
1	A	105	PRO
4	T	96	GLY
4	I	97	GLY
5	U	52	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	234/234 (100%)	224 (96%)	10 (4%)	35 66
1	F	234/234 (100%)	228 (97%)	6 (3%)	54 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	234/234 (100%)	225 (96%)	9 (4%)	40	71
1	Q	234/234 (100%)	226 (97%)	8 (3%)	44	75
2	B	94/94 (100%)	91 (97%)	3 (3%)	46	77
2	G	94/94 (100%)	91 (97%)	3 (3%)	46	77
2	L	94/94 (100%)	88 (94%)	6 (6%)	22	47
2	R	94/94 (100%)	91 (97%)	3 (3%)	46	77
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	7 (78%)	2 (22%)	1	3
3	M	9/9 (100%)	7 (78%)	2 (22%)	1	3
3	S	9/9 (100%)	7 (78%)	2 (22%)	1	3
4	D	163/164 (99%)	155 (95%)	8 (5%)	31	61
4	I	164/164 (100%)	154 (94%)	10 (6%)	23	49
4	N	164/164 (100%)	158 (96%)	6 (4%)	41	72
4	T	164/164 (100%)	154 (94%)	10 (6%)	23	49
5	E	213/213 (100%)	198 (93%)	15 (7%)	19	42
5	J	213/213 (100%)	201 (94%)	12 (6%)	26	54
5	P	213/213 (100%)	204 (96%)	9 (4%)	36	68
5	U	213/213 (100%)	199 (93%)	14 (7%)	21	45
All	All	2855/2856 (100%)	2717 (95%)	138 (5%)	31	62

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	35	ARG
1	A	44	ARG
1	A	69	THR
1	A	102	ASP
1	A	110	LEU
1	A	141	GLN
1	A	183	ASP
1	A	226	GLN
1	A	239	ARG
2	B	55	SER
2	B	70	PHE
2	B	83	ASN

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Mol	Chain	Res	Type
4	D	2	ASN
4	D	61	ARG
4	D	77	LEU
4	D	85	SER
4	D	132	LYS
4	D	133	SER
4	D	184	LYS
4	D	191	ASN
5	E	1	ASP
5	E	56	ASP
5	E	62	ASP
5	E	79	LEU
5	E	118	GLU
5	E	138	ILE
5	E	146	LEU
5	E	149	LEU
5	E	174	CYS
5	E	180	LEU
5	E	186	LEU
5	E	196	ARG
5	E	221	SER
5	E	229	ASP
5	E	245	ARG
1	F	35	ARG
1	F	71	THR
1	F	154	GLU
1	F	186	LYS
1	F	226	GLN
1	F	239	ARG
2	G	3	ARG
2	G	45	ARG
2	G	83	ASN
3	H	8	LEU
3	H	9	THR
4	I	2	ASN
4	I	32	LEU
4	I	80	LEU
4	I	81	GLN
4	I	85	SER
4	I	87	SER
4	I	136	LYS
4	I	155	ASP

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Mol	Chain	Res	Type
4	I	164	CYS
4	I	186	ASP
5	J	12	VAL
5	J	60	VAL
5	J	66	SER
5	J	76	LEU
5	J	79	LEU
5	J	113	ARG
5	J	114	LEU
5	J	167	LYS
5	J	180	LEU
5	J	222	GLU
5	J	228	GLN
5	J	245	ARG
1	K	69	THR
1	K	81	LEU
1	K	106	ASP
1	K	138	THR
1	K	180	GLN
1	K	181	ARG
1	K	196	ASP
1	K	206	LEU
1	K	275	GLU
2	L	1	ILE
2	L	38	ASP
2	L	53	ASP
2	L	54	LEU
2	L	70	PHE
2	L	97	ARG
3	M	3	LEU
3	M	9	THR
4	N	1	GLN
4	N	3	ILE
4	N	4	ASP
4	N	85	SER
4	N	186	ASP
4	N	194	ASN
5	P	62	ASP
5	P	79	LEU
5	P	121	ASN
5	P	160	LEU
5	P	171	SER

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Mol	Chain	Res	Type
5	P	174	CYS
5	P	180	LEU
5	P	196	ARG
5	P	208	ARG
1	Q	17	ARG
1	Q	21	ARG
1	Q	23	ILE
1	Q	81	LEU
1	Q	82	ARG
1	Q	110	LEU
1	Q	156	LEU
1	Q	253	GLU
2	R	31	HIS
2	R	34	ASP
2	R	83	ASN
3	S	3	LEU
3	S	9	THR
4	T	1	GLN
4	T	8	THR
4	T	26	THR
4	T	80	LEU
4	T	87	SER
4	T	136	LYS
4	T	148	THR
4	T	150	VAL
4	T	157	ASP
4	T	184	LYS
5	U	5	THR
5	U	25	GLN
5	U	53	LYS
5	U	59	GLU
5	U	67	VAL
5	U	79	LEU
5	U	113	ARG
5	U	121	ASN
5	U	167	LYS
5	U	180	LEU
5	U	187	ASN
5	U	198	ARG
5	U	202	THR
5	U	245	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	80	ASN
1	A	141	GLN
1	A	174	ASN
1	A	226	GLN
1	A	260	HIS
1	A	263	HIS
2	B	83	ASN
4	D	5	GLN
4	D	21	ASN
4	D	30	ASN
4	D	38	HIS
4	D	93	GLN
4	D	119	GLN
4	D	149	ASN
4	D	152	GLN
4	D	183	ASN
4	D	191	ASN
5	E	6	GLN
5	E	28	ASN
5	E	47	HIS
5	E	187	ASN
5	E	228	GLN
1	F	3	HIS
1	F	65	GLN
1	F	80	ASN
1	F	155	GLN
1	F	180	GLN
1	F	197	HIS
1	F	260	HIS
1	F	263	HIS
2	G	17	ASN
2	G	83	ASN
4	I	5	GLN
4	I	21	ASN
4	I	30	ASN
4	I	38	HIS
4	I	81	GLN
4	I	93	GLN
4	I	115	HIS
4	I	183	ASN
5	J	6	GLN

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Mol	Chain	Res	Type
5	J	10	HIS
5	J	106	GLN
5	J	121	ASN
5	J	157	HIS
5	J	209	ASN
5	J	228	GLN
1	K	80	ASN
1	K	127	ASN
1	K	180	GLN
1	K	242	GLN
1	K	255	GLN
1	K	263	HIS
2	L	83	ASN
4	N	1	GLN
4	N	5	GLN
4	N	21	ASN
4	N	38	HIS
4	N	49	ASN
4	N	93	GLN
5	P	106	GLN
5	P	228	GLN
1	Q	3	HIS
1	Q	32	GLN
1	Q	65	GLN
1	Q	80	ASN
1	Q	155	GLN
1	Q	260	HIS
1	Q	263	HIS
2	R	51	HIS
2	R	83	ASN
4	T	1	GLN
4	T	5	GLN
4	T	21	ASN
4	T	38	HIS
4	T	127	GLN
5	U	6	GLN
5	U	28	ASN
5	U	106	GLN
5	U	157	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.