



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:42 AM UTC

PDB ID : 2NX5 / pdb_00002nx5
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

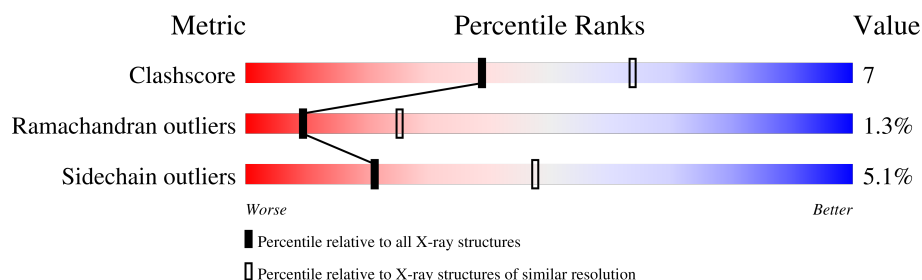
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	276	82% 18%
1	F	276	82% 17% .
1	K	276	85% 13% .
1	Q	276	78% 21%
2	B	99	93% 7%
2	G	99	88% 12%
2	L	99	86% 11% .
2	R	99	80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	11	 55% 45%
3	H	11	 36% 36% 27%
3	M	11	 45% 36% 18%
3	S	11	 36% 55% 9%
4	D	188	 75% 20% 5%
4	I	188	 76% 21% . .
4	N	188	 75% 21% .
4	T	188	 76% 21% . .
5	E	243	 81% 15% .
5	J	243	 83% 16%
5	P	243	 81% 17% .
5	U	243	 79% 19% .

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		

Continued on next page...

Continued from previous page...

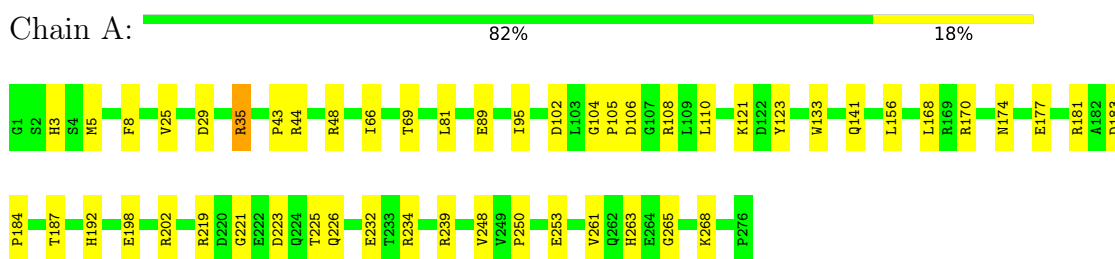
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	14	Total 14	O 14	0	0
6	L	6	Total 6	O 6	0	0
6	N	16	Total 16	O 16	0	0
6	P	20	Total 20	O 20	0	0
6	Q	15	Total 15	O 15	0	0
6	R	5	Total 5	O 5	0	0
6	T	10	Total 10	O 10	0	0
6	U	10	Total 10	O 10	0	0

3 Residue-property plots

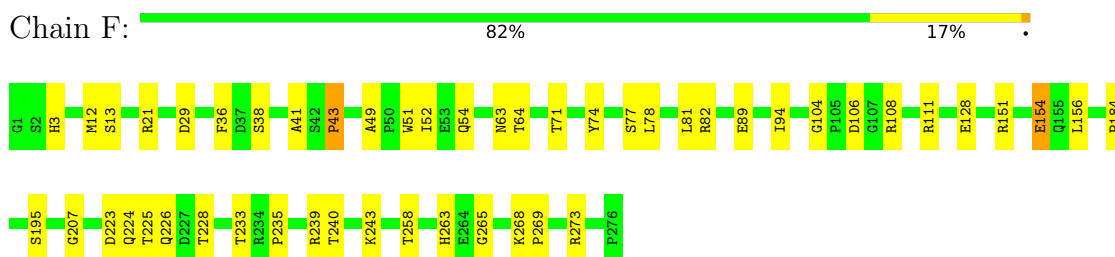
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

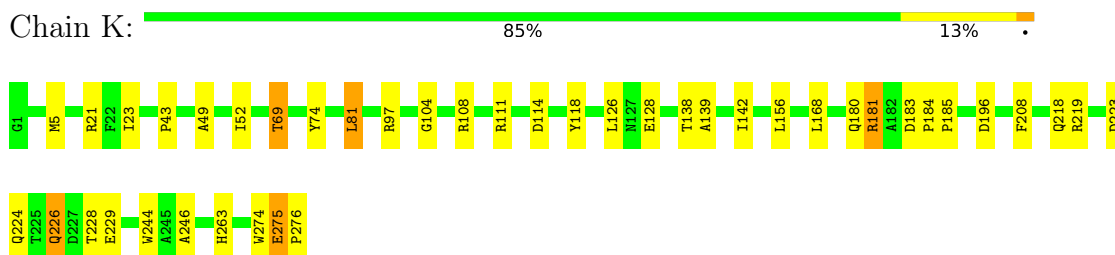
• Molecule 1: HLA-B35



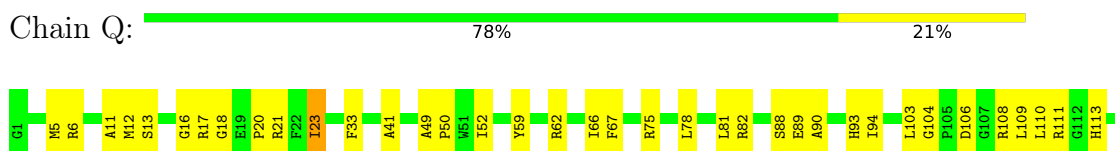
• Molecule 1: HLA-B35

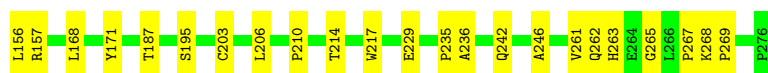


• Molecule 1: HLA-B35



• Molecule 1: HLA-B35

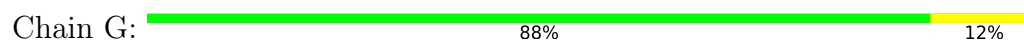




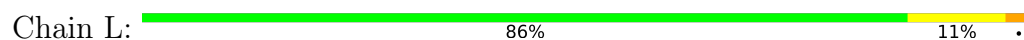
- Molecule 2: Beta-2-microglobulin



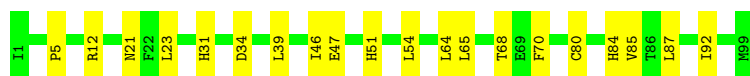
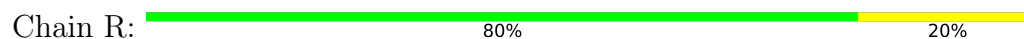
- Molecule 2: Beta-2-microglobulin



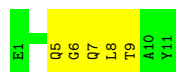
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: EBV peptide, EPLPQGQLTAY



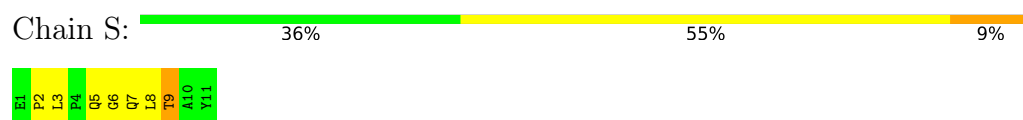
- Molecule 3: EBV peptide, EPLPQGQLTAY



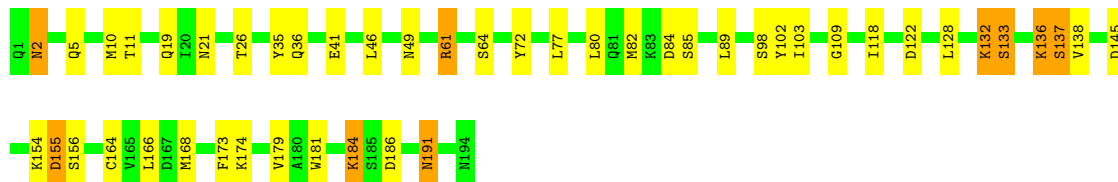
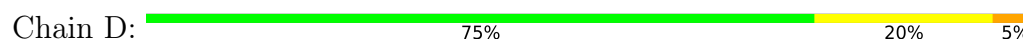
- Molecule 3: EBV peptide, EPLPQGQLTAY



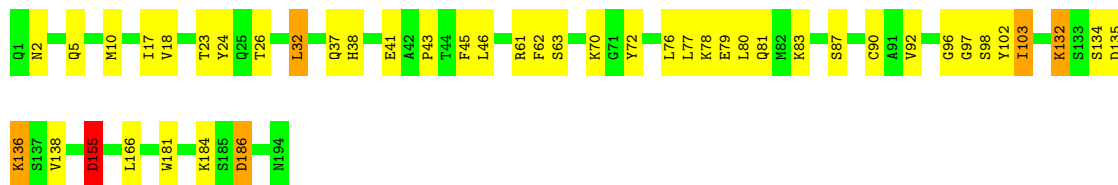
- Molecule 3: EBV peptide, EPLPQGQLTAY



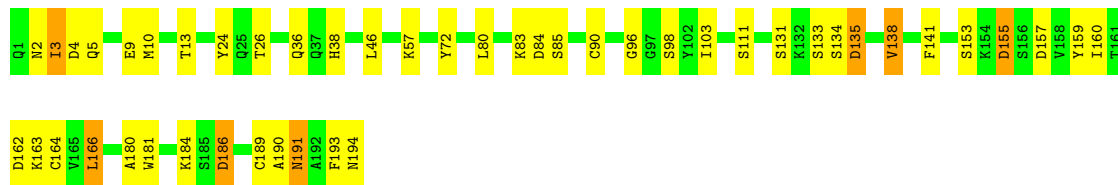
- Molecule 4: ELS4 TCR alpha chain



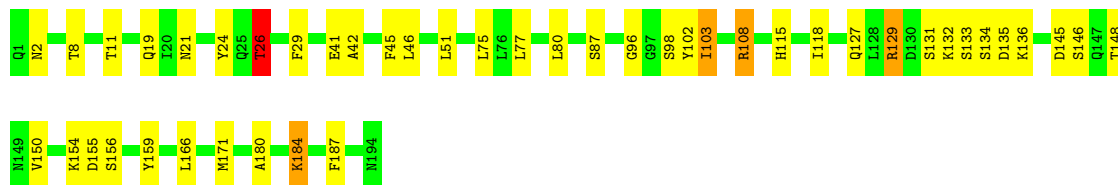
- Molecule 4: ELS4 TCR alpha chain



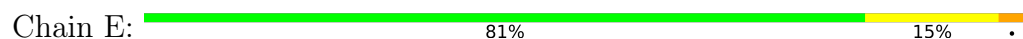
- Molecule 4: ELS4 TCR alpha chain



- Molecule 4: ELS4 TCR alpha chain



- Molecule 5: ELS4 TCR beta chain





- Molecule 5: ELS4 TCR beta chain

Chain J: 83% 16%



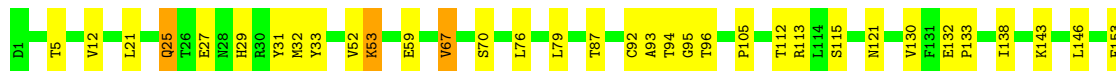
- Molecule 5: ELS4 TCR beta chain

Chain P: 81% 17%



- Molecule 5: ELS4 TCR beta chain

Chain U: 79% 19%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/2317	0.74	0/3150
1	F	0.42	0/2317	0.75	0/3150
1	K	0.43	0/2317	0.76	2/3150 (0.1%)
1	Q	0.43	0/2317	0.73	0/3150
2	B	0.40	0/852	0.67	0/1152
2	G	0.42	0/852	0.69	0/1152
2	L	0.41	0/852	0.70	0/1152
2	R	0.44	0/852	0.71	0/1152
3	C	0.54	0/88	0.92	0/119
3	H	0.57	0/88	0.92	0/119
3	M	0.51	0/88	0.68	0/119
3	S	0.50	0/88	0.89	0/119
4	D	0.42	0/1498	0.81	5/2027 (0.2%)
4	I	0.43	0/1499	0.76	0/2028
4	N	0.45	0/1499	0.77	0/2028
4	T	0.43	0/1499	0.77	1/2028 (0.0%)
5	E	0.41	0/1989	0.72	2/2707 (0.1%)
5	J	0.40	0/1989	0.75	0/2707
5	P	0.42	0/1989	0.72	0/2707
5	U	0.42	0/1989	0.73	0/2707
All	All	0.42	0/26979	0.74	10/36623 (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
4	D	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	137	SER	N-CA-C	7.60	121.87	109.94
5	E	183	GLN	CA-C-N	6.44	126.67	119.32
5	E	183	GLN	C-N-CA	6.44	126.67	119.32
4	T	26	THR	N-CA-C	6.27	118.67	108.26
4	D	132	LYS	CA-C-N	5.44	131.48	121.70
4	D	132	LYS	C-N-CA	5.44	131.48	121.70
1	K	104	GLY	CA-C-N	5.27	126.42	119.84
1	K	104	GLY	C-N-CA	5.27	126.42	119.84
4	D	136	LYS	N-CA-C	5.19	118.25	108.65
4	D	26	THR	N-CA-C	5.09	116.61	107.80

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	22	0
1	F	2254	0	2117	31	0
1	K	2254	0	2117	26	0
1	Q	2254	0	2117	36	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	28	0
4	I	1467	0	1387	27	0
4	N	1467	0	1387	25	0
4	T	1467	0	1387	36	0
5	E	1936	0	1817	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	1936	0	1817	21	0
5	P	1936	0	1817	33	0
5	U	1936	0	1817	30	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
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	347	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 (347) 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:HG3	5:P:208:ARG:HH11	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:HH11	4:T:108:ARG:HG2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:HIS:CD2	1:F:265:GLY:H	2.03	0.77
4:D:10:MET:HE1	4:D:19:GLN:O	1.87	0.74
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:HG3	5:P:208:ARG:NH1	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
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
1:A:104:GLY:C	1:A:106:ASP:H	2.05	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
1:Q:88:SER:C	1:Q:90:ALA:H	2.06	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:D:154:LYS:C	4:D:156:SER:H	2.08	0.62
2:G:36:GLU:O	2:G:82:VAL:HA	2.00	0.61
4:T:24:TYR:HD1	4:T:26:THR:HG22	1.64	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:I:98:SER:C	4:I:103:ILE:H	2.11	0.58
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:D:98:SER:C	4:D:103:ILE:H	2.11	0.57
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
5:P:53:LYS:HE2	5:P:53:LYS:HA	1.86	0.57
2:R:84:HIS:H	2:R:87:LEU:HD12	1.69	0.57
4:D:128:LEU:O	4:D:137:SER:HB2	2.04	0.57
3:S:7:GLN:HB2	5:U:96:THR:HB	1.85	0.57
2:L:1:ILE:HG12	2:L:2:GLN:HG3	1.87	0.57
5:P:121:ASN:HA	5:P:226:TRP:HZ3	1.70	0.57
5:E:220:LEU:O	5:E:221:SER:CB	2.53	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
3:H:7:GLN:C	3:H:9:THR:H	2.12	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: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:Q:13:SER:HB3	1:Q:93:HIS:H	1.70	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
4:D:191:ASN:C	4:D:191:ASN:HD22	2.14	0.55
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:D:98:SER:O	4:D:103:ILE:N	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:98:SER:C	4:T:103:ILE:H	2.15	0.54
4:T:129:ARG:HH21	4:T:129:ARG:CG	2.11	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
3:M:7:GLN:C	3:M:9:THR:H	2.15	0.54
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
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
5:P:208:ARG:HH11	5:P:208:ARG:CG	2.05	0.53
4:T:131:SER:HB2	5:U:132:GLU:HG2	1.89	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
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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:53:LYS:HE2	5:U:70:SER:HA	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
2:R:46:ILE:HG21	2:R:68:THR:HG21	1.92	0.50
1:Q:23:ILE:HD13	2:R:54:LEU:HD23	1.93	0.50
4:T:127:GLN:HE21	4:T:129:ARG:HH22	1.60	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
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:Q:187:THR:HG21	1:Q:261:VAL:HG21	1.94	0.49
1:F:21:ARG:HG3	1:F:38:SER:OG	2.12	0.49
4:N:131:SER:HB2	5:P:132:GLU:HG3	1.93	0.49
1:Q:206:LEU:HD23	1:Q:242:GLN:HB2	1.94	0.49
2:R:21:ASN:HB3	2:R:70:PHE:CE1	2.47	0.49
4:I:38:HIS:HE1	4:I:83:LYS:O	1.96	0.49
4:I:184:LYS:HG2	4:I:186:ASP:H	1.76	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
1:F:77:SER:HB3	3:M:11:TYR:HB2	1.95	0.48
2:R:51:HIS:HD2	2:R:64:LEU:HD22	1.77	0.48
4:T:154:LYS:C	4:T:156:SER:H	2.21	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:NH1	5:P:208:ARG:CG	2.71	0.48
5:P:153:PHE:HE1	5:P:156:ASP:HA	1.78	0.48
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.96	0.48
5:P:46:ILE:HG22	5:P:47:HIS:CD2	2.49	0.48
1:F:226:GLN:C	1:F:228:THR:H	2.21	0.48
1:F:51:TRP:O	1:F:54:GLN:HG2	2.14	0.47
1:K:229:GLU:N	1:K:246:ALA:O	2.43	0.47
1:A:8:PHE:HB2	1:A:25:VAL:HG23	1.95	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: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
2:B:21:ASN:CG	2:B:22:PHE:H	2.22	0.47
4:N:184:LYS:HE3	4:N:186:ASP:HB2	1.96	0.47
1:A:133:TRP:HH2	1:A:156:LEU:CD1	2.28	0.47
2:B:13:HIS:H	2:B:21:ASN:HD21	1.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:38:HIS:HB2	4:I:41:GLU:HG2	1.96	0.47
4:I:138:VAL:HG22	4:I:181:TRP:HB3	1.97	0.47
1:Q:33:PHE:CD2	1:Q:52:ILE:HD13	2.49	0.47
4:I:18:VAL:HG12	4:I:77:LEU:HB2	1.97	0.47
1:A:219:ARG:C	1:A:221:GLY:H	2.23	0.47
2:G:59:ASP:O	2:G:60:TRP:HB2	2.15	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:T:108:ARG:NH1	4:T:108:ARG:CG	2.76	0.46
4:D:61:ARG:HH22	4:D:84:ASP:CG	2.23	0.46
4:D:118:ILE:HG13	4:D:145:ASP:HA	1.97	0.46
1:K:5:MET:HB2	1:K:168:LEU:HD13	1.97	0.46
4:N:166:LEU:HB3	5:P:174:CYS:HB3	1.97	0.46
2:G:17:ASN:HD21	2:G:74:GLU:HG3	1.80	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: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
4:I:70:LYS:HE2	4:N:72:TYR:CG	2.50	0.46
5:J:23:CYS:HB2	5:J:34:TRP:CZ2	2.51	0.46
4:N:138:VAL:HG22	4:N:181:TRP:HB3	1.97	0.46
5:U:87:THR:HG23	5:U:115:SER:HA	1.97	0.46
4:D:5:GLN:NE2	4:D:109:GLY:H	2.14	0.46
2:L:12:ARG:HE	2:L:22:PHE:HB2	1.81	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
1:Q:268:LYS:HG3	1:Q:269:PRO:HD2	1.97	0.46
1:A:104:GLY:C	1:A:106:ASP:N	2.73	0.46
4:D:36:GLN:HB2	4:D:46:LEU:HD11	1.98	0.46
1:F:223:ASP:HB3	1:F:225:THR:HG23	1.98	0.46
4:I:134:SER:O	4:I:135:ASP:HB2	2.15	0.46
1:Q:59:TYR:OH	1:Q:171:TYR:OH	2.33	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:J:87:THR:HG23	5:J:115:SER:HA	1.99	0.45
1:K:208:PHE:CD2	1:K:263:HIS:HE1	2.34	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:A:3:HIS:HD2	1:A:29:ASP:OD2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:98:SER:C	4:N:103:ILE:H	2.25	0.45
5:P:121:ASN:HA	5:P:226:TRP:CZ3	2.52	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
5:P:36:ARG:HH12	5:P:86:GLN:HA	1.81	0.45
1:Q:59:TYR:HH	1:Q:171:TYR:HH	1.59	0.45
4:T:24:TYR:CD1	4:T:26:THR:CG2	2.98	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
5:E:221:SER:OG	5:E:222:GLU:HA	2.17	0.45
3:H:6:GLY:HA2	5:P:30:ARG:NH2	2.30	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
4:T:133:SER:O	4:T:134:SER:HB3	2.17	0.44
1:F:106:ASP:OD2	1:F:108:ARG:N	2.36	0.44
3:S:6:GLY:O	3:S:9:THR:HG22	2.17	0.44
5:U:204:TRP:C	5:U:206:ASN:H	2.26	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:D:98:SER:C	4:D:103:ILE:N	2.76	0.44
1:A:250:PRO:O	1:A:253:GLU:HB2	2.18	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
3:M:3:LEU:HD23	3:M:5:GLN:CG	2.48	0.43
1:Q:67:PHE:CZ	3:S:2:PRO:HB3	2.53	0.43
4:T:132:LYS:HG2	5:U:240:ALA:CB	2.47	0.43
5:U:25:GLN:HG2	5:U:27:GLU:H	1.82	0.43
2:G:71:THR:HA	2:G:72:PRO:HD3	1.86	0.43
1:Q:104:GLY:C	1:Q:106:ASP:H	2.26	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
5:E:11:LYS:HD2	5:E:13:THR:HG23	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
2:R:39:LEU:HD13	2:R:68:THR:HG22	2.00	0.43
1:A:202:ARG:HD2	6:B:100:HOH:O	2.19	0.43
4:D:82:MET:CG	4:D:174:LYS:HE2	2.48	0.43
4:I:5:GLN:HE22	4:I:90:CYS:H	1.65	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:69:ARG:HG3	5:J:69:ARG:O	2.17	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
1:K:226:GLN:C	1:K:228:THR:H	2.25	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
4:D:154:LYS:C	4:D:156:SER:N	2.77	0.43
1:Q:16:GLY:C	1:Q:18:GLY:H	2.27	0.43
1:F:36:PHE:HE2	1:F:64:THR:HG23	1.84	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
5:U:33:TYR:O	5:U:92:CYS:HA	2.19	0.43
5:E:29:HIS:HB3	5:E:95:GLY:O	2.19	0.43
4:I:186:ASP:OD2	4:I:186:ASP:N	2.52	0.43
1:K:184:PRO:HA	1:K:185:PRO:HD3	1.93	0.43
1:Q:6:ARG:HH12	1:Q:113:HIS:HB2	1.84	0.43
1:F:268:LYS:HD2	1:F:269:PRO:HD2	2.01	0.42
4:I:45:PHE:CD1	5:J:105:PRO:HB3	2.54	0.42
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
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:46:ILE:O	5:E:61:SER:OG	2.33	0.42
5:E:156:ASP:HB2	5:E:179:PRO:HG2	2.01	0.42
4:D:155:ASP:HB3	1:F:184:PRO:HG2	2.02	0.42
4:N:155:ASP:C	4:N:157:ASP:H	2.28	0.42
5:U:25:GLN:OE1	5:U:29:HIS:N	2.50	0.42
5:U:138:ILE:HG23	5:U:201:ALA:HB1	2.01	0.42
5:P:17:THR:HA	5:P:18:PRO:HD3	1.93	0.42
1:Q:236:ALA:O	2:R:12:ARG:HG3	2.18	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: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:K:74:TYR:OH	1:K:97:ARG:HD3	2.19	0.42
1:Q:103:LEU:HD23	1:Q:109:LEU:HA	2.01	0.42
2:R:80:CYS:O	2:R:92:ILE:HA	2.20	0.42
1:K:219:ARG:HB2	1:K:224:GLN:HG3	2.02	0.42
4:N:3:ILE:H	4:N:3:ILE:HG12	1.58	0.42
5:U:153:PHE:HE1	5:U:156:ASP:HA	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HE2	1:A:121:LYS:HB3	1.83	0.41
5:E:65:TYR:CD1	5:E:79:LEU:HD22	2.55	0.41
5:P:155:PRO:HG2	5:P:157:HIS:CD2	2.55	0.41
1:Q:214:THR:HB	1:Q:262:GLN:HB2	2.01	0.41
4:T:118:ILE:HG13	4:T:145:ASP:HA	2.01	0.41
5:U:187:ASN:OD1	5:U:187:ASN:N	2.53	0.41
5:J:36:ARG:NH1	5:J:65:TYR:OH	2.53	0.41
1:Q:157:ARG:HG2	4:T:51:LEU:HD21	2.02	0.41
3:C:7:GLN:O	5:E:98:ASP:OD2	2.37	0.41
5:E:32:MET:HG2	5:E:94:THR:HG22	2.01	0.41
1:F:104:GLY:C	1:F:106:ASP:H	2.28	0.41
4:I:37:GLN:HB2	4:I:43:PRO:HB3	2.01	0.41
1:K:139:ALA:HA	1:K:142:ILE:HD12	2.02	0.41
2:R:5:PRO:HG3	2:R:84:HIS:HB2	2.02	0.41
5:U:130:VAL:HG23	5:U:240:ALA:HB3	2.03	0.41
5:U:212:ARG:NH1	5:U:214:GLN:OE1	2.51	0.41
1:A:35:ARG:HG2	1:A:48:ARG:HD3	2.02	0.41
2:R:84:HIS:CE1	2:R:85:VAL:HG12	2.56	0.41
5:U:67:VAL:HA	5:U:76:LEU:O	2.20	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
1:K:208:PHE:CD2	1:K:263:HIS:CE1	3.09	0.41
3:M:7:GLN:O	3:M:9:THR:N	2.52	0.41
4:N:36:GLN:HB2	4:N:46:LEU:HD11	2.02	0.41
4:T:46:LEU:HD13	4:T:75:LEU:HD21	2.02	0.41
5:E:214:GLN:HG3	5:E:237:ILE:CG2	2.51	0.41
4:I:10:MET:HE2	1:K:108:ARG:HH22	1.84	0.41
1:Q:49:ALA:HA	1:Q:50:PRO:HD3	1.92	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
1:A:108:ARG:NH1	4:T:11:THR:O	2.54	0.41
1:K:181:ARG:HH21	1:K:183:ASP:N	2.19	0.41
2:L:97:ARG:HD2	2:L:97:ARG:H	1.86	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
5:E:6:GLN:HE21	5:E:109:GLY:HA3	1.86	0.40
5:U:113:ARG:HB3	5:U:113:ARG:HH11	1.86	0.40
4:D:122:ASP:OD2	1:Q:269:PRO:HG2	2.22	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:164:CYS:HB2	6:P:248:HOH:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:6:ARG:HH22	1:Q:113:HIS:CD2	2.38	0.40
1:F:224:GLN:C	1:F:226:GLN:H	2.28	0.40
1:F:108:ARG:NH2	4:N:10:MET:HE2	2.36	0.40
5:P:7:SER:HA	5:P:8:PRO:HA	1.89	0.40
4:I:61:ARG:NH1	4:I:79:GLU:O	2.54	0.40
4:N:162:ASP:OD1	4:N:163:LYS:N	2.53	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%)	18	41
1	F	274/276 (99%)	254 (93%)	18 (7%)	2 (1%)	18	41
1	K	274/276 (99%)	258 (94%)	14 (5%)	2 (1%)	18	41
1	Q	274/276 (99%)	255 (93%)	15 (6%)	4 (2%)	8	22
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%)	12	32
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%)	5	14
4	I	186/188 (99%)	167 (90%)	13 (7%)	6 (3%)	3	7
4	N	186/188 (99%)	160 (86%)	19 (10%)	7 (4%)	2	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	T	186/188 (99%)	168 (90%)	13 (7%)	5 (3%)	4	10
5	E	241/243 (99%)	229 (95%)	10 (4%)	2 (1%)	16	37
5	J	241/243 (99%)	233 (97%)	8 (3%)	0	100	100
5	P	241/243 (99%)	227 (94%)	12 (5%)	2 (1%)	16	37
5	U	241/243 (99%)	227 (94%)	12 (5%)	2 (1%)	16	37
All	All	3228/3268 (99%)	3009 (93%)	177 (6%)	42 (1%)	9	25

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	220 (94%)	14 (6%)	17	41
1	F	234/234 (100%)	229 (98%)	5 (2%)	47	75
1	K	234/234 (100%)	227 (97%)	7 (3%)	36	66
1	Q	234/234 (100%)	226 (97%)	8 (3%)	32	62
2	B	94/94 (100%)	93 (99%)	1 (1%)	65	85
2	G	94/94 (100%)	93 (99%)	1 (1%)	65	85
2	L	94/94 (100%)	88 (94%)	6 (6%)	16	38
2	R	94/94 (100%)	91 (97%)	3 (3%)	34	64
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	6 (67%)	3 (33%)	0	1
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%)	153 (94%)	10 (6%)	17	40
4	I	164/164 (100%)	154 (94%)	10 (6%)	17	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	N	164/164 (100%)	156 (95%)	8 (5%)	22	49
4	T	164/164 (100%)	152 (93%)	12 (7%)	13	32
5	E	213/213 (100%)	196 (92%)	17 (8%)	11	28
5	J	213/213 (100%)	201 (94%)	12 (6%)	19	44
5	P	213/213 (100%)	202 (95%)	11 (5%)	21	47
5	U	213/213 (100%)	198 (93%)	15 (7%)	14	34
All	All	2855/2856 (100%)	2708 (95%)	147 (5%)	21	48

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	44	ARG
1	A	66	ILE
1	A	69	THR
1	A	89	GLU
1	A	102	ASP
1	A	110	LEU
1	A	141	GLN
1	A	183	ASP
1	A	192	HIS
1	A	226	GLN
1	A	232	GLU
1	A	239	ARG
1	A	268	LYS
2	B	55	SER
4	D	2	ASN
4	D	41	GLU
4	D	61	ARG
4	D	77	LEU
4	D	80	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	11	LYS
5	E	56	ASP
5	E	62	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	222	GLU
5	E	237	ILE
5	E	245	ARG
1	F	63	ASN
1	F	71	THR
1	F	81	LEU
1	F	154	GLU
1	F	156	LEU
2	G	77	GLU
3	H	3	LEU
3	H	8	LEU
3	H	9	THR
4	I	17	ILE
4	I	32	LEU
4	I	80	LEU
4	I	81	GLN
4	I	87	SER
4	I	103	ILE
4	I	132	LYS
4	I	136	LYS
4	I	155	ASP
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	145	THR
5	J	167	LYS
5	J	186	LEU
5	J	222	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	J	228	GLN
5	J	245	ARG
1	K	69	THR
1	K	81	LEU
1	K	138	THR
1	K	180	GLN
1	K	181	ARG
1	K	196	ASP
1	K	275	GLU
2	L	1	ILE
2	L	38	ASP
2	L	53	ASP
2	L	54	LEU
2	L	58	LYS
2	L	97	ARG
3	M	3	LEU
3	M	9	THR
4	N	3	ILE
4	N	4	ASP
4	N	57	LYS
4	N	85	SER
4	N	138	VAL
4	N	166	LEU
4	N	186	ASP
4	N	194	ASN
5	P	11	LYS
5	P	19	VAL
5	P	62	ASP
5	P	79	LEU
5	P	117	LEU
5	P	121	ASN
5	P	160	LEU
5	P	171	SER
5	P	174	CYS
5	P	180	LEU
5	P	208	ARG
1	Q	12	MET
1	Q	17	ARG
1	Q	23	ILE
1	Q	81	LEU
1	Q	82	ARG
1	Q	94	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	110	LEU
1	Q	156	LEU
2	R	31	HIS
2	R	34	ASP
2	R	47	GLU
3	S	3	LEU
3	S	9	THR
4	T	8	THR
4	T	26	THR
4	T	77	LEU
4	T	80	LEU
4	T	87	SER
4	T	103	ILE
4	T	108	ARG
4	T	129	ARG
4	T	136	LYS
4	T	148	THR
4	T	150	VAL
4	T	184	LYS
5	U	5	THR
5	U	12	VAL
5	U	25	GLN
5	U	53	LYS
5	U	59	GLU
5	U	67	VAL
5	U	79	LEU
5	U	121	ASN
5	U	160	LEU
5	U	167	LYS
5	U	180	LEU
5	U	187	ASN
5	U	198	ARG
5	U	202	THR
5	U	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	226	GLN
1	A	255	GLN
1	A	260	HIS
2	B	13	HIS
2	B	42	ASN
2	B	83	ASN
4	D	1	GLN
4	D	5	GLN
4	D	19	GLN
4	D	21	ASN
4	D	30	ASN
4	D	37	GLN
4	D	38	HIS
4	D	119	GLN
4	D	120	ASN
4	D	147	GLN
4	D	149	ASN
4	D	183	ASN
4	D	191	ASN
5	E	6	GLN
5	E	28	ASN
5	E	37	GLN
5	E	47	HIS
5	E	121	ASN
5	E	183	GLN
5	E	187	ASN
5	E	228	GLN
1	F	3	HIS
1	F	63	ASN
1	F	80	ASN
1	F	155	GLN
1	F	180	GLN
1	F	192	HIS
1	F	197	HIS
1	F	260	HIS
1	F	263	HIS
2	G	13	HIS
2	G	17	ASN
2	G	83	ASN
4	I	21	ASN
4	I	30	ASN
4	I	37	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	I	38	HIS
4	I	49	ASN
4	I	81	GLN
4	I	93	GLN
4	I	115	HIS
4	I	127	GLN
4	I	183	ASN
5	J	10	HIS
5	J	37	GLN
5	J	106	GLN
5	J	187	ASN
5	J	209	ASN
5	J	228	GLN
1	K	80	ASN
1	K	87	GLN
1	K	127	ASN
1	K	144	GLN
1	K	224	GLN
1	K	242	GLN
1	K	255	GLN
1	K	263	HIS
2	L	13	HIS
2	L	83	ASN
4	N	1	GLN
4	N	5	GLN
4	N	19	GLN
4	N	21	ASN
4	N	25	GLN
4	N	30	ASN
4	N	38	HIS
4	N	49	ASN
5	P	121	ASN
5	P	157	HIS
5	P	165	ASN
5	P	187	ASN
5	P	228	GLN
1	Q	3	HIS
1	Q	32	GLN
1	Q	65	GLN
1	Q	80	ASN
1	Q	144	GLN
1	Q	155	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	191	HIS
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
4	T	147	GLN
5	U	6	GLN
5	U	24	HIS
5	U	28	ASN
5	U	47	HIS
5	U	106	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.