



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:20 AM UTC

PDB ID : 3PQY / pdb_00003pqy
Title : Crystal Structure of 6218 TCR in complex with the H2Db-PA224
Authors : Gras, S.; Guillonneau, C.; Turner, S.J.; Rossjohn, J.
Deposited on : 2010-11-28
Resolution : 3.19 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

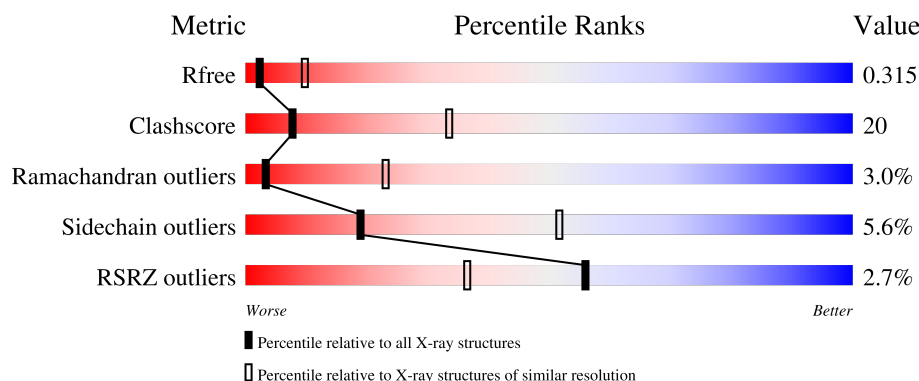
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	275	 61% 37% .
1	F	275	 64% 32% ..
1	K	275	 64% 32% .
1	P	275	 67% 30% ..
2	B	99	 62% 35% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	99	% 51% 44% . .
2	L	99	% 55% 42% ..
2	Q	99	% 65% 34% .
3	C	10	30% 60% 10%
3	H	10	70% 30%
3	M	10	70% 30%
3	R	10	50% 40% 10%
4	D	195	7% 59% 28% 8% . .
4	I	195	3% 51% 37% 7% . .
4	N	195	6% 43% 38% 8% 11%
4	S	195	7% 52% 31% 6% . 11%
5	E	240	65% 30% 5%
5	J	240	% 50% 46% .
5	O	240	60% 37% .
5	T	240	% 52% 41% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25956 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	1	0	0
			2260	1428	399	424	9			
1	F	267	Total	C	N	O	S	1	0	0
			2198	1391	389	409	9			
1	K	275	Total	C	N	O	S	0	0	0
			2260	1428	399	424	9			
1	P	273	Total	C	N	O	S	1	0	0
			2244	1418	397	420	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			
2	G	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			
2	L	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			
2	Q	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ASP	ALA	variant	UNP P01887
G	85	ASP	ALA	variant	UNP P01887
L	85	ASP	ALA	variant	UNP P01887
Q	85	ASP	ALA	variant	UNP P01887

- Molecule 3 is a protein called 10-mer peptide from RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			84	53	14	17			
3	H	10	Total	C	N	O	0	0	0
			84	53	14	17			
3	M	10	Total	C	N	O	0	0	0
			84	53	14	17			
3	R	10	Total	C	N	O	0	0	0
			84	53	14	17			

- Molecule 4 is a protein called T cell receptor alpha variable 21-DV12,T-cell receptor, sp3.4 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	189	Total	C	N	O	S	0	0	0
			1464	916	244	295	9			
4	I	188	Total	C	N	O	S	0	0	0
			1464	918	243	294	9			
4	N	174	Total	C	N	O	S	0	0	0
			1350	846	226	269	9			
4	S	174	Total	C	N	O	S	0	0	0
			1348	845	225	269	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	107	SER	-	linker	UNP A0A075B6C4
D	108	GLY	-	linker	UNP A0A075B6C4
D	109	GLY	-	linker	UNP A0A075B6C4
D	110	SER	-	linker	UNP A0A075B6C4
D	111	ASN	-	linker	UNP A0A075B6C4
D	112	TYR	-	linker	UNP A0A075B6C4
D	113	LYS	-	linker	UNP A0A075B6C4
D	114	LEU	-	linker	UNP A0A075B6C4
D	115	THR	-	linker	UNP A0A075B6C4
D	116	PHE	-	linker	UNP A0A075B6C4
D	117	GLY	-	linker	UNP A0A075B6C4
D	118	LYS	-	linker	UNP A0A075B6C4
D	119	GLY	-	linker	UNP A0A075B6C4
D	120	THR	-	linker	UNP A0A075B6C4
D	121	LEU	-	linker	UNP A0A075B6C4
D	122	LEU	-	linker	UNP A0A075B6C4
D	123	THR	-	linker	UNP A0A075B6C4
D	124	VAL	-	linker	UNP A0A075B6C4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	125	THR	-	linker	UNP A0A075B6C4
D	126	PRO	-	linker	UNP A0A075B6C4
I	107	SER	-	linker	UNP A0A075B6C4
I	108	GLY	-	linker	UNP A0A075B6C4
I	109	GLY	-	linker	UNP A0A075B6C4
I	110	SER	-	linker	UNP A0A075B6C4
I	111	ASN	-	linker	UNP A0A075B6C4
I	112	TYR	-	linker	UNP A0A075B6C4
I	113	LYS	-	linker	UNP A0A075B6C4
I	114	LEU	-	linker	UNP A0A075B6C4
I	115	THR	-	linker	UNP A0A075B6C4
I	116	PHE	-	linker	UNP A0A075B6C4
I	117	GLY	-	linker	UNP A0A075B6C4
I	118	LYS	-	linker	UNP A0A075B6C4
I	119	GLY	-	linker	UNP A0A075B6C4
I	120	THR	-	linker	UNP A0A075B6C4
I	121	LEU	-	linker	UNP A0A075B6C4
I	122	LEU	-	linker	UNP A0A075B6C4
I	123	THR	-	linker	UNP A0A075B6C4
I	124	VAL	-	linker	UNP A0A075B6C4
I	125	THR	-	linker	UNP A0A075B6C4
I	126	PRO	-	linker	UNP A0A075B6C4
N	107	SER	-	linker	UNP A0A075B6C4
N	108	GLY	-	linker	UNP A0A075B6C4
N	109	GLY	-	linker	UNP A0A075B6C4
N	110	SER	-	linker	UNP A0A075B6C4
N	111	ASN	-	linker	UNP A0A075B6C4
N	112	TYR	-	linker	UNP A0A075B6C4
N	113	LYS	-	linker	UNP A0A075B6C4
N	114	LEU	-	linker	UNP A0A075B6C4
N	115	THR	-	linker	UNP A0A075B6C4
N	116	PHE	-	linker	UNP A0A075B6C4
N	117	GLY	-	linker	UNP A0A075B6C4
N	118	LYS	-	linker	UNP A0A075B6C4
N	119	GLY	-	linker	UNP A0A075B6C4
N	120	THR	-	linker	UNP A0A075B6C4
N	121	LEU	-	linker	UNP A0A075B6C4
N	122	LEU	-	linker	UNP A0A075B6C4
N	123	THR	-	linker	UNP A0A075B6C4
N	124	VAL	-	linker	UNP A0A075B6C4
N	125	THR	-	linker	UNP A0A075B6C4
N	126	PRO	-	linker	UNP A0A075B6C4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	107	SER	-	linker	UNP A0A075B6C4
S	108	GLY	-	linker	UNP A0A075B6C4
S	109	GLY	-	linker	UNP A0A075B6C4
S	110	SER	-	linker	UNP A0A075B6C4
S	111	ASN	-	linker	UNP A0A075B6C4
S	112	TYR	-	linker	UNP A0A075B6C4
S	113	LYS	-	linker	UNP A0A075B6C4
S	114	LEU	-	linker	UNP A0A075B6C4
S	115	THR	-	linker	UNP A0A075B6C4
S	116	PHE	-	linker	UNP A0A075B6C4
S	117	GLY	-	linker	UNP A0A075B6C4
S	118	LYS	-	linker	UNP A0A075B6C4
S	119	GLY	-	linker	UNP A0A075B6C4
S	120	THR	-	linker	UNP A0A075B6C4
S	121	LEU	-	linker	UNP A0A075B6C4
S	122	LEU	-	linker	UNP A0A075B6C4
S	123	THR	-	linker	UNP A0A075B6C4
S	124	VAL	-	linker	UNP A0A075B6C4
S	125	THR	-	linker	UNP A0A075B6C4
S	126	PRO	-	linker	UNP A0A075B6C4

- Molecule 5 is a protein called T cell receptor beta, variable 29,Human nkt tcr beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			
5	J	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			
5	O	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			
5	T	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	108	PHE	-	linker	UNP A0A0G2LB96
E	109	GLY	-	linker	UNP A0A0G2LB96
E	110	ARG	-	linker	UNP A0A0G2LB96
E	123	LEU	THR	conflict	UNP K7N5M4
J	108	PHE	-	linker	UNP A0A0G2LB96
J	109	GLY	-	linker	UNP A0A0G2LB96

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	110	ARG	-	linker	UNP A0A0G2LB96
J	123	LEU	THR	conflict	UNP K7N5M4
O	108	PHE	-	linker	UNP A0A0G2LB96
O	109	GLY	-	linker	UNP A0A0G2LB96
O	110	ARG	-	linker	UNP A0A0G2LB96
O	123	LEU	THR	conflict	UNP K7N5M4
T	108	PHE	-	linker	UNP A0A0G2LB96
T	109	GLY	-	linker	UNP A0A0G2LB96
T	110	ARG	-	linker	UNP A0A0G2LB96
T	123	LEU	THR	conflict	UNP K7N5M4

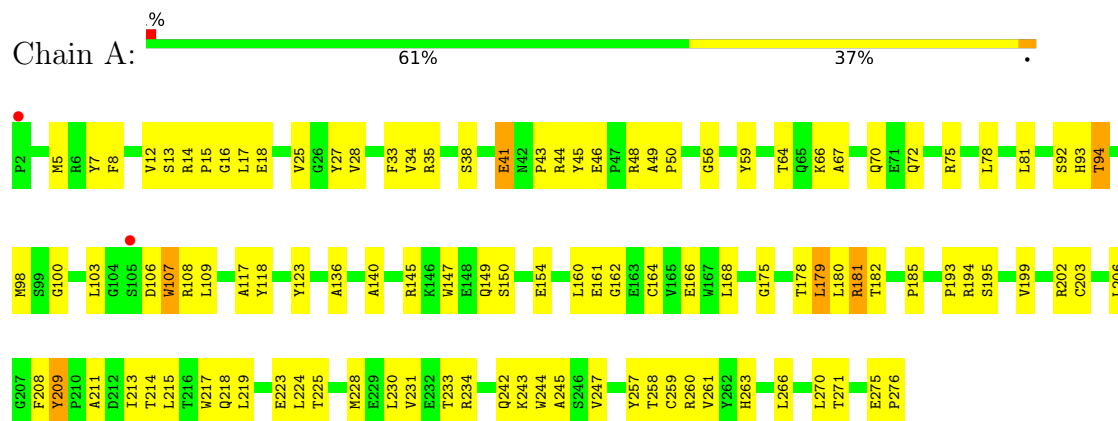
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	B	2	Total O 2 2	0	0
6	D	1	Total O 1 1	0	0
6	E	2	Total O 2 2	0	0
6	J	1	Total O 1 1	0	0
6	K	1	Total O 1 1	0	0
6	N	1	Total O 1 1	0	0
6	O	2	Total O 2 2	0	0
6	P	2	Total O 2 2	0	0
6	R	1	Total O 1 1	0	0
6	S	1	Total O 1 1	0	0

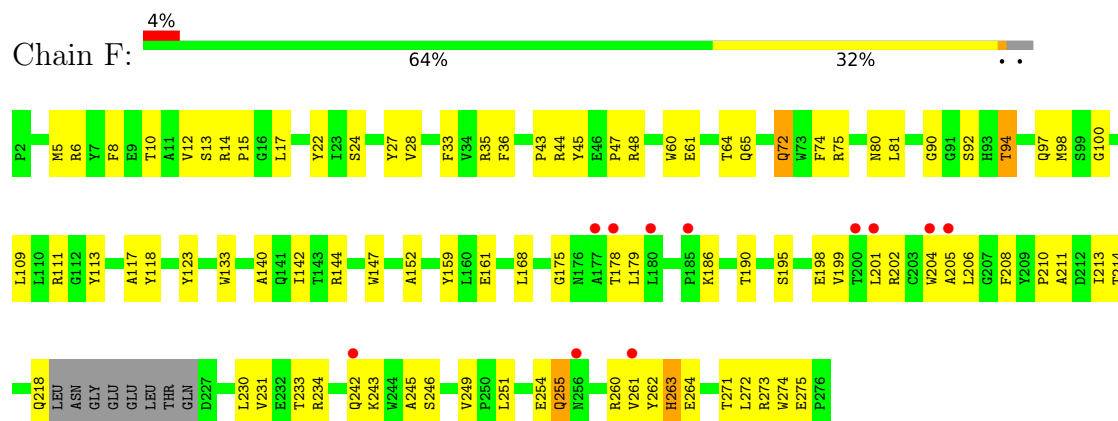
3 Residue-property plots [i](#)

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

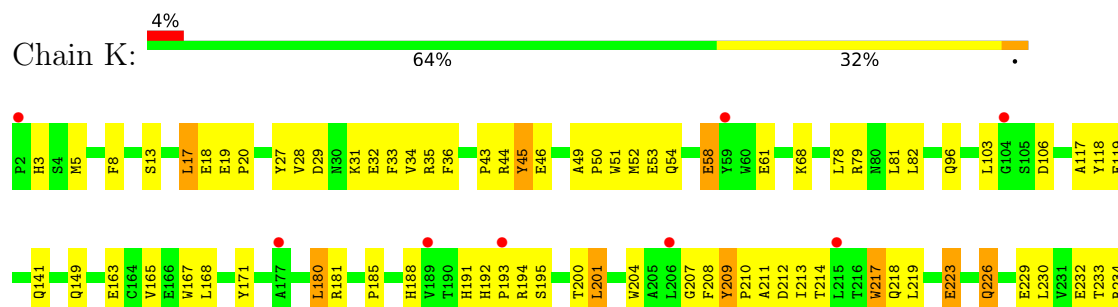
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

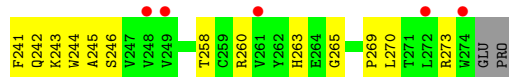
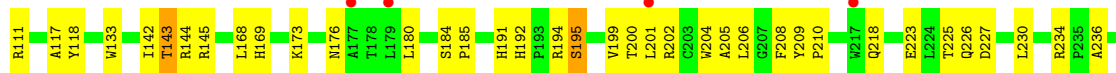


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

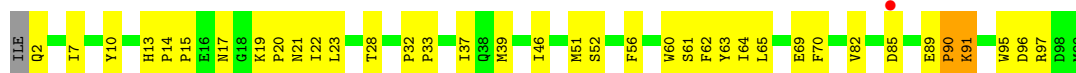




- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



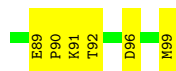
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

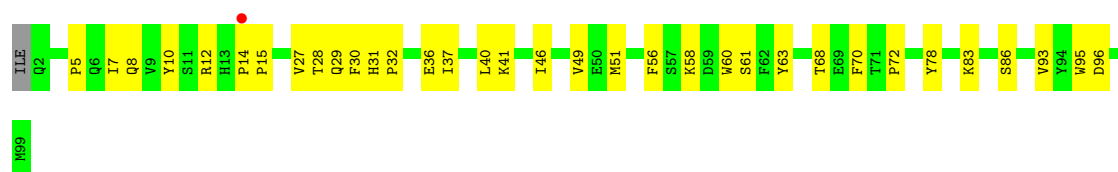


- Molecule 2: Beta-2-microglobulin

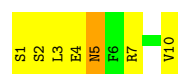


- Molecule 2: Beta-2-microglobulin

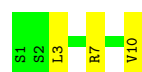




- Molecule 3: 10-mer peptide from RNA-directed RNA polymerase



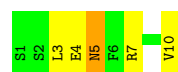
- Molecule 3: 10-mer peptide from RNA-directed RNA polymerase



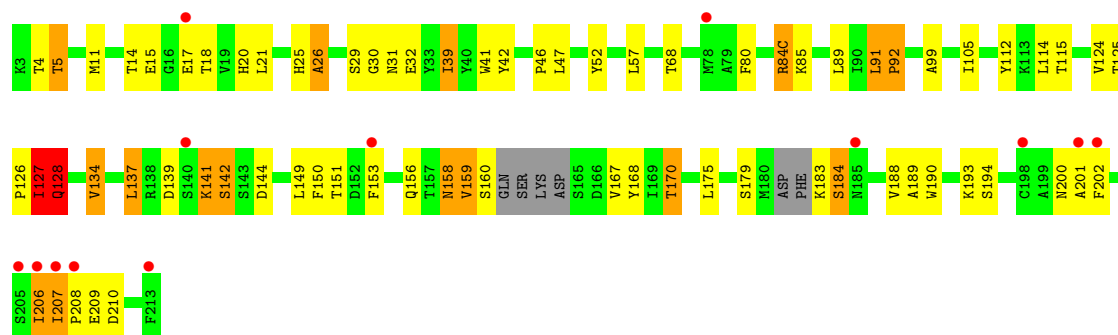
- Molecule 3: 10-mer peptide from RNA-directed RNA polymerase



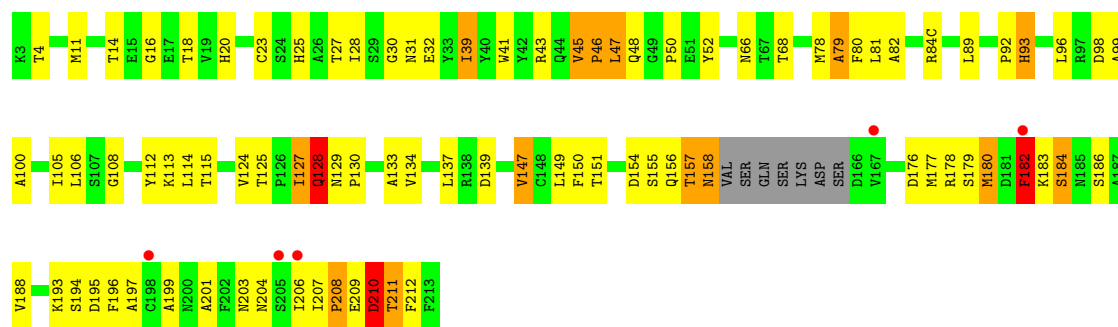
- Molecule 3: 10-mer peptide from RNA-directed RNA polymerase



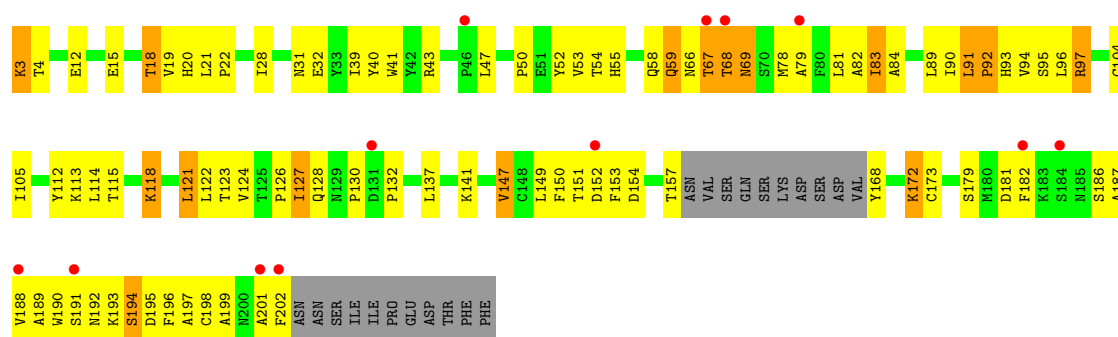
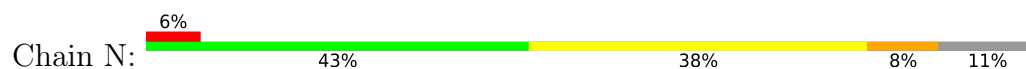
- Molecule 4: T cell receptor alpha variable 21-DV12,T-cell receptor, sp3.4 alpha chain



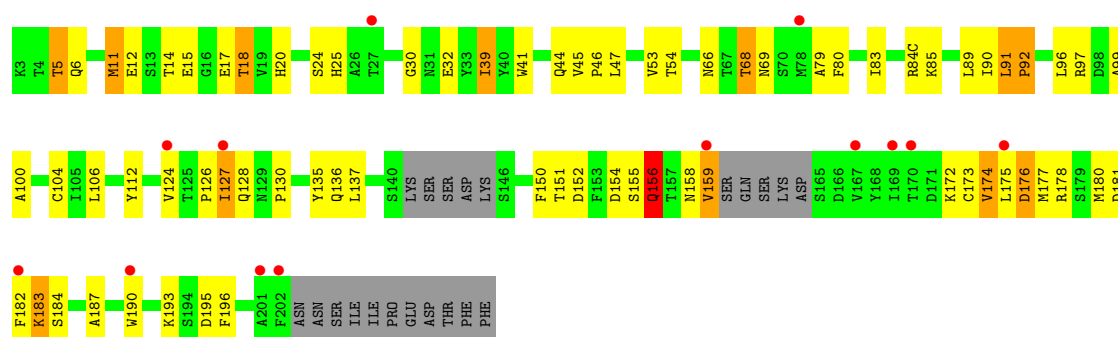
- Molecule 4: T cell receptor alpha variable 21-DV12,T-cell receptor, sp3.4 alpha chain



- Molecule 4: T cell receptor alpha variable 21-DV12,T-cell receptor, sp3.4 alpha chain

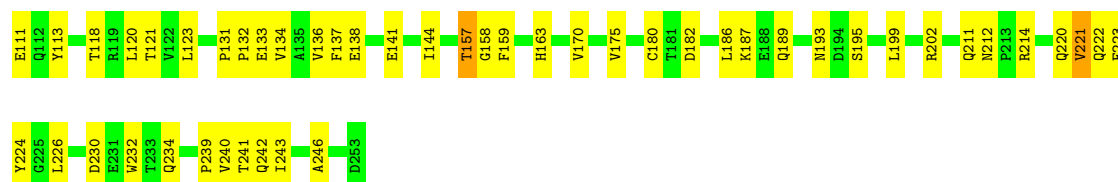


- Molecule 4: T cell receptor alpha variable 21-DV12,T-cell receptor, sp3.4 alpha chain

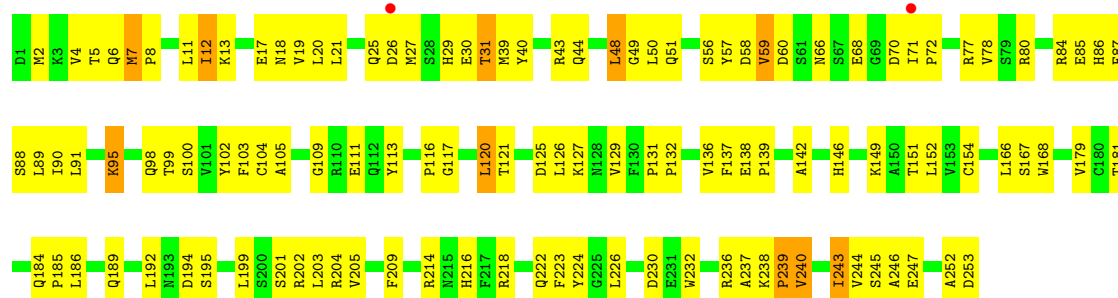


- Molecule 5: T cell receptor beta, variable 29,Human nkt tcr beta chain





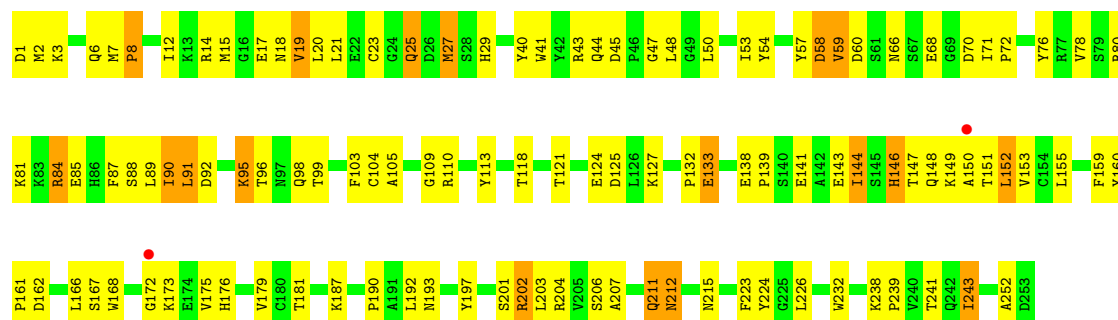
- Molecule 5: T cell receptor beta, variable 29, Human nkt tcr beta chain



- Molecule 5: T cell receptor beta, variable 29, Human nkt tcr beta chain



- Molecule 5: T cell receptor beta, variable 29, Human nkt tcr beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.89Å 199.06Å 202.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 3.19 49.61 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.61-3.19) 97.4 (49.61-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.19Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.6.1_357	Depositor
R, R_{free}	0.246 , 0.316 0.242 , 0.315	Depositor DCC
R_{free} test set	3545 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25956	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2923e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.25	0/2327	0.68	0/3160
1	F	0.25	0/2264	0.65	0/3073
1	K	0.25	0/2327	0.65	0/3160
1	P	0.25	0/2310	0.68	0/3136
2	B	0.25	0/839	0.74	0/1137
2	G	0.26	0/839	0.64	0/1137
2	L	0.25	0/839	0.73	0/1137
2	Q	0.25	0/839	0.73	0/1137
3	C	0.25	0/85	0.59	0/112
3	H	0.22	0/85	0.52	0/112
3	M	0.23	0/85	0.52	0/112
3	R	0.21	0/85	0.55	0/112
4	D	0.27	0/1495	0.72	3/2032 (0.1%)
4	I	0.26	0/1497	0.71	0/2036
4	N	0.28	0/1380	0.69	1/1875 (0.1%)
4	S	0.26	0/1377	0.70	2/1873 (0.1%)
5	E	0.26	0/1992	0.68	2/2702 (0.1%)
5	J	0.25	0/1992	0.68	0/2702
5	O	0.26	0/1992	0.67	0/2702
5	T	0.25	0/1992	0.68	0/2702
All	All	0.25	0/26641	0.68	8/36149 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	91	LEU	CA-C-N	5.34	126.52	119.84
4	S	91	LEU	C-N-CA	5.34	126.52	119.84
4	N	182	PHE	CB-CA-C	-5.21	110.58	116.63
5	E	189	GLN	CA-C-N	5.20	125.50	119.47
5	E	189	GLN	C-N-CA	5.20	125.50	119.47
4	D	84(C)	ARG	CB-CA-C	-5.15	109.66	115.79
4	D	91	LEU	CA-C-N	5.05	126.16	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	91	LEU	C-N-CA	5.05	126.16	119.84

There are no chirality outliers.

There are no planarity outliers.

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	2260	0	2131	78	0
1	F	2198	0	2072	68	0
1	K	2260	0	2133	74	0
1	P	2244	0	2118	69	0
2	B	813	0	782	28	0
2	G	813	0	782	37	0
2	L	813	0	782	35	0
2	Q	813	0	782	24	0
3	C	84	0	80	8	0
3	H	84	0	80	3	0
3	M	84	0	80	2	0
3	R	84	0	80	5	0
4	D	1464	0	1399	75	0
4	I	1464	0	1394	102	0
4	N	1350	0	1294	85	0
4	S	1348	0	1286	67	0
5	E	1941	0	1857	65	0
5	J	1941	0	1857	99	0
5	O	1941	0	1857	78	0
5	T	1941	0	1857	117	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	D	1	0	0	0	0
6	E	2	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	N	1	0	0	0	0
6	O	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	2	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
All	All	25956	0	24703	1010	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 20.

All (1010) 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:S:183:LYS:HB2	4:S:184:SER:HB2	1.38	1.03
4:S:30:GLY:HA2	4:S:84(C):ARG:HH12	1.22	1.02
5:E:7:MET:HB3	5:E:8:PRO:HD2	1.43	1.00
5:J:59:VAL:HG13	5:J:60:ASP:H	1.30	0.96
5:T:7:MET:HB3	5:T:8:PRO:HD2	1.45	0.95
5:T:99:THR:HG23	5:T:121:THR:HA	1.48	0.94
5:O:2:MET:HE1	5:O:29:HIS:CE1	2.04	0.93
4:D:206:ILE:HG13	4:D:207:ILE:H	1.32	0.92
4:D:207:ILE:HG13	4:D:209:GLU:H	1.34	0.92
5:E:2:MET:HE1	5:E:29:HIS:HE1	1.35	0.91
2:G:29:GLN:HA	2:G:61:SER:HB3	1.54	0.89
4:D:99:ALA:HB2	4:D:124:VAL:HG12	1.55	0.88
5:O:2:MET:HE1	5:O:29:HIS:HE1	1.33	0.88
4:D:175:LEU:HB3	5:E:180:CYS:HB2	1.57	0.86
5:J:6:GLN:NE2	5:J:104:CYS:H	1.73	0.86
5:J:19:VAL:HB	5:J:91:LEU:HB2	1.56	0.85
5:E:2:MET:HE1	5:E:29:HIS:CE1	2.12	0.85
1:P:6:ARG:HH11	1:P:6:ARG:HG2	1.42	0.85
1:A:266:LEU:HD21	1:A:270:LEU:HG	1.58	0.85
4:I:99:ALA:HB2	4:I:124:VAL:HG22	1.60	0.83
1:P:97:GLN:HE22	3:R:5:ASN:HD21	1.23	0.83
1:F:218:GLN:HE22	1:F:260:ARG:HH11	1.24	0.83
5:O:99:THR:HG23	5:O:121:THR:HA	1.59	0.82
5:O:44:GLN:HB2	5:O:50:LEU:HD23	1.62	0.82
4:N:50:PRO:HG3	5:O:50:LEU:HD11	1.61	0.82
4:S:173:CYS:HB2	5:T:202:ARG:HH11	1.45	0.82
5:E:43:ARG:HH21	5:E:100:SER:HB2	1.43	0.82
5:E:19:VAL:HB	5:E:91:LEU:HB2	1.63	0.81
4:N:95:SER:HB3	4:N:97:ARG:HH11	1.44	0.80
1:P:6:ARG:HH11	1:P:6:ARG:CG	1.94	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:163:HIS:HB3	5:E:224:TYR:HB2	1.64	0.79
5:O:66:ASN:HD22	5:O:78:VAL:HG23	1.46	0.79
4:S:69:ASN:HD21	4:S:79:ALA:HB3	1.48	0.79
1:F:142:ILE:HD11	1:P:142:ILE:HD11	1.65	0.79
1:K:213:ILE:HG12	1:K:214:THR:H	1.50	0.77
2:L:73:THR:HG22	2:L:74:GLU:H	1.50	0.77
1:K:13:SER:HA	1:K:20:PRO:HB3	1.65	0.77
1:K:230:LEU:HD11	1:K:243:LYS:HE3	1.67	0.76
5:T:6:GLN:NE2	5:T:104:CYS:H	1.82	0.76
4:N:150:PHE:HB3	4:N:153:PHE:HE2	1.50	0.76
5:J:99:THR:HG23	5:J:121:THR:HA	1.67	0.75
4:N:66:ASN:ND2	4:N:67:THR:H	1.84	0.75
4:S:183:LYS:CB	4:S:184:SER:HB2	2.16	0.74
1:F:202:ARG:HG2	1:F:246:SER:HB3	1.68	0.74
5:E:7:MET:HB3	5:E:8:PRO:CD	2.17	0.74
5:J:7:MET:HB3	5:J:8:PRO:HD3	1.69	0.74
4:D:20:HIS:CE1	4:I:20:HIS:HE1	2.06	0.73
2:L:33:PRO:HG3	2:L:62:PHE:CZ	2.24	0.72
4:S:135:TYR:CZ	5:T:143:GLU:HG2	2.23	0.72
5:T:207:ALA:O	5:T:211:GLN:HG2	1.88	0.72
2:B:13:HIS:HB2	2:B:21:ASN:HD21	1.55	0.72
5:O:6:GLN:NE2	5:O:104:CYS:H	1.88	0.72
5:T:19:VAL:HG22	5:T:91:LEU:HD11	1.70	0.72
4:I:179:SER:HA	4:I:180:MET:HB2	1.72	0.71
5:O:68:GLU:HB3	5:O:72:PRO:HG3	1.73	0.71
4:N:150:PHE:HB3	4:N:153:PHE:CE2	2.26	0.71
5:T:152:LEU:HD13	5:T:152:LEU:H	1.55	0.71
3:R:7:ARG:HD2	5:T:109:GLY:O	1.91	0.70
4:I:133:ALA:HA	4:I:211:THR:HG22	1.73	0.70
5:O:144:ILE:HG23	5:O:207:ALA:HB1	1.72	0.70
4:D:150:PHE:HB3	4:D:153:PHE:CE1	2.26	0.70
4:S:127:ILE:HD12	4:S:127:ILE:H	1.56	0.70
4:N:147:VAL:HG23	4:N:190:TRP:HB3	1.72	0.70
5:O:40:TYR:HB2	5:O:105:ALA:HB3	1.74	0.69
4:I:179:SER:HB2	4:I:180:MET:O	1.93	0.69
4:N:118:LYS:HE2	4:N:118:LYS:HA	1.74	0.69
5:T:20:LEU:HD13	5:T:90:ILE:HG23	1.73	0.69
5:T:7:MET:CB	5:T:8:PRO:HD2	2.22	0.68
5:T:149:LYS:HB3	5:T:206:SER:HA	1.73	0.68
1:P:230:LEU:HD11	1:P:243:LYS:HE3	1.74	0.68
5:E:25:GLN:HG3	5:E:27:MET:H	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:45:VAL:HG22	4:I:46:PRO:HD2	1.75	0.68
5:O:19:VAL:HB	5:O:91:LEU:HB2	1.76	0.67
2:Q:95:TRP:CD1	2:Q:96:ASP:H	2.12	0.67
1:A:231:VAL:O	1:A:243:LYS:HE3	1.94	0.67
1:P:218:GLN:HG2	1:P:223:GLU:HG2	1.77	0.67
5:J:7:MET:HB3	5:J:8:PRO:CD	2.25	0.67
4:D:144:ASP:HB3	4:D:194:SER:HB3	1.75	0.67
4:D:206:ILE:HG23	4:D:207:ILE:HG23	1.77	0.67
4:I:178:ARG:N	4:I:179:SER:HB3	2.08	0.67
5:T:66:ASN:HD22	5:T:78:VAL:HG23	1.60	0.67
1:A:180:LEU:HD12	1:A:181:ARG:N	2.09	0.67
1:P:204:TRP:HE3	1:P:206:LEU:HD11	1.60	0.67
4:D:105:ILE:HG21	4:D:114:LEU:HB2	1.77	0.66
5:T:151:THR:OG1	5:T:204:ARG:HA	1.94	0.66
3:C:10:VAL:HG12	3:C:10:VAL:O	1.94	0.66
5:J:189:GLN:HB3	5:J:192:LEU:HD13	1.77	0.66
5:T:25:GLN:HE22	5:T:29:HIS:N	1.92	0.66
1:K:238:ASP:HB3	2:L:12:ARG:HH21	1.60	0.66
2:L:42:ASN:HD21	2:L:76:ASP:HA	1.60	0.66
4:S:130:PRO:HB3	4:S:154:ASP:HB2	1.76	0.66
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.30	0.66
3:H:7:ARG:HD2	5:J:109:GLY:O	1.96	0.66
2:Q:29:GLN:HA	2:Q:61:SER:HB3	1.77	0.66
5:O:15:MET:HE3	5:O:96:THR:HG23	1.76	0.66
1:P:13:SER:O	1:P:92:SER:HA	1.96	0.66
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.31	0.65
4:I:176:ASP:CG	4:I:177:MET:H	2.03	0.65
5:J:59:VAL:HG13	5:J:60:ASP:N	2.09	0.65
4:N:153:PHE:H	4:N:154:ASP:HA	1.59	0.65
1:F:72:GLN:HG2	1:F:75:ARG:HH12	1.60	0.65
5:T:15:MET:HE3	5:T:96:THR:HG23	1.78	0.65
5:T:68:GLU:HB3	5:T:72:PRO:HG3	1.79	0.65
2:G:5:PRO:HB3	2:G:30:PHE:HB3	1.79	0.65
4:N:188:VAL:HG23	5:O:202:ARG:HH21	1.61	0.65
4:D:20:HIS:HE1	4:I:20:HIS:HE1	1.43	0.65
1:K:235:PRO:HG2	2:L:65:LEU:HD22	1.79	0.65
5:J:216:HIS:HE1	5:J:247:GLU:HB2	1.62	0.65
1:A:5:MET:HE3	1:A:7:TYR:HE2	1.60	0.64
4:N:151:THR:HG22	4:N:186:SER:HB3	1.77	0.64
5:J:77:ARG:HB3	5:J:90:ILE:HB	1.78	0.64
1:P:192:HIS:HB2	1:P:200:THR:HG23	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:209:GLU:N	4:I:210:ASP:HB3	2.12	0.64
4:N:69:ASN:HB2	4:N:79:ALA:O	1.97	0.64
2:L:40:LEU:HD21	2:L:81:ARG:HH21	1.60	0.64
5:O:55:ILE:HG22	5:O:67:SER:HB2	1.79	0.64
5:O:136:VAL:HG23	5:O:246:ALA:HB3	1.80	0.64
4:D:29:SER:HB2	4:D:32:GLU:HG3	1.78	0.64
5:E:11:LEU:HD23	5:E:120:LEU:HD13	1.78	0.64
4:D:206:ILE:CG1	4:D:207:ILE:H	2.08	0.64
4:I:203:ASN:HB3	4:I:204:ASN:HB3	1.80	0.64
4:N:19:VAL:HG21	4:N:122:LEU:HD21	1.80	0.64
1:K:229:GLU:HB3	1:K:246:SER:HB3	1.80	0.64
5:T:40:TYR:HB2	5:T:105:ALA:HB3	1.80	0.64
1:P:57:PRO:HA	1:P:60:TRP:HD1	1.63	0.63
4:I:14:THR:HG22	4:I:125:THR:HB	1.80	0.63
1:K:207:GLY:HA2	1:K:240:THR:HB	1.80	0.63
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.80	0.63
4:I:177:MET:HB2	4:I:179:SER:HB3	1.81	0.63
4:I:179:SER:HA	4:I:180:MET:CB	2.29	0.63
4:S:175:LEU:HB2	4:S:184:SER:HB3	1.79	0.63
5:E:70:ASP:C	5:E:72:PRO:HD3	2.24	0.63
5:O:110:ARG:HG2	5:O:111:GLU:HG3	1.81	0.63
5:T:143:GLU:OE1	5:T:150:ALA:HB2	1.98	0.63
4:N:66:ASN:CG	4:N:67:THR:H	2.05	0.63
1:A:12:VAL:HG22	1:A:94:THR:HG23	1.80	0.62
1:F:28:VAL:HG23	1:F:33:PHE:CE2	2.34	0.62
5:O:189:GLN:O	5:O:192:LEU:HB2	1.99	0.62
5:J:95:LYS:HE3	5:J:95:LYS:HA	1.81	0.62
1:A:223:GLU:HG2	1:P:176:ASN:HD21	1.63	0.62
4:I:25:HIS:HB2	4:I:106:LEU:HD11	1.82	0.62
5:E:59:VAL:O	5:E:80:ARG:HB3	2.00	0.62
4:S:99:ALA:HB2	4:S:124:VAL:HG12	1.82	0.62
2:B:33:PRO:HG3	2:B:62:PHE:CE1	2.34	0.62
4:D:52:TYR:CB	5:E:111:GLU:HG3	2.30	0.62
4:N:153:PHE:H	4:N:154:ASP:CA	2.12	0.62
5:E:2:MET:HE2	5:E:113:TYR:CZ	2.35	0.62
2:L:50:GLU:HB2	2:L:67:HIS:CE1	2.35	0.62
1:A:230:LEU:HD13	1:A:245:ALA:HB2	1.82	0.61
2:G:13:HIS:HB2	2:G:14:PRO:HD2	1.82	0.61
4:I:193:LYS:HG2	4:I:195:ASP:H	1.65	0.61
5:E:214:ARG:HE	5:E:214:ARG:HA	1.65	0.61
1:K:79:ARG:HH12	5:O:59:VAL:HG23	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:226:LEU:HD13	5:T:239:PRO:HG2	1.82	0.61
1:F:231:VAL:O	1:F:243:LYS:HE3	2.00	0.61
1:A:217:TRP:H	1:A:228:MET:HE1	1.65	0.61
5:O:68:GLU:HB3	5:O:72:PRO:CG	2.29	0.61
5:O:166:LEU:HD23	5:O:167:SER:N	2.15	0.61
5:O:14:ARG:HB2	5:O:126:LEU:HD11	1.82	0.61
5:E:2:MET:HE2	5:E:113:TYR:CE1	2.35	0.61
2:L:56:PHE:HB3	2:L:62:PHE:CD2	2.35	0.61
1:P:236:ALA:HB1	2:Q:12:ARG:HG3	1.81	0.61
4:S:41:TRP:O	4:S:53:VAL:HG22	2.00	0.61
5:T:21:LEU:HD12	5:T:89:LEU:HD23	1.81	0.61
5:J:2:MET:HG3	5:J:113:TYR:CE1	2.36	0.61
5:J:25:GLN:O	5:J:26:ASP:HB2	1.99	0.61
1:K:28:VAL:HG23	1:K:33:PHE:CE1	2.36	0.61
4:S:80:PHE:HB2	4:S:90:ILE:HB	1.81	0.61
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.36	0.61
4:D:156:GLN:HG3	4:D:158:ASN:ND2	2.16	0.61
1:F:263:HIS:CG	1:F:264:GLU:H	2.19	0.61
4:S:183:LYS:HB2	4:S:184:SER:CB	2.24	0.61
5:E:20:LEU:HD23	5:E:90:ILE:HG13	1.83	0.60
5:O:2:MET:HE2	5:O:113:TYR:CD1	2.35	0.60
1:F:6:ARG:HB2	1:F:27:TYR:HB2	1.82	0.60
5:J:70:ASP:C	5:J:72:PRO:HD3	2.26	0.60
4:D:29:SER:C	4:D:31:ASN:H	2.10	0.60
2:L:11:SER:HB2	2:L:21:ASN:HD21	1.65	0.60
5:T:105:ALA:HA	5:T:113:TYR:O	2.00	0.60
4:I:30:GLY:HA2	4:I:84(C):ARG:HH12	1.67	0.60
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.84	0.60
5:J:238:LYS:HE3	5:J:240:VAL:HG21	1.82	0.60
4:I:96:LEU:HA	4:I:124:VAL:HG21	1.82	0.60
4:I:183:LYS:HG2	4:I:184:SER:N	2.17	0.60
1:K:234:ARG:HD2	2:L:8:GLN:NE2	2.16	0.60
4:N:19:VAL:HG23	4:N:94:VAL:HG11	1.83	0.60
4:I:45:VAL:HG23	4:I:100:ALA:HB2	1.83	0.60
4:S:53:VAL:HG23	4:S:54:THR:HG22	1.83	0.60
5:J:179:VAL:HG22	5:J:203:LEU:HD13	1.84	0.60
2:G:27:VAL:HG21	2:G:37:ILE:HD12	1.84	0.59
4:I:178:ARG:H	4:I:179:SER:HB3	1.67	0.59
4:I:130:PRO:HG3	4:I:154:ASP:HB2	1.84	0.59
2:L:96:ASP:HB3	2:L:99:MET:HB2	1.84	0.59
4:N:153:PHE:N	4:N:154:ASP:HA	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:THR:HG21	4:I:68:THR:HB	1.85	0.59
4:D:170:THR:CG2	4:D:188:VAL:H	2.15	0.59
5:J:166:LEU:HD23	5:J:167:SER:N	2.17	0.59
4:S:30:GLY:HA2	4:S:84(C):ARG:NH1	2.05	0.59
5:T:25:GLN:NE2	5:T:29:HIS:H	2.01	0.59
1:F:80:ASN:HA	1:P:86:ASN:HD21	1.68	0.59
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.37	0.59
4:I:78:MET:O	4:I:79:ALA:HB3	2.02	0.59
5:J:48:LEU:H	5:J:48:LEU:HD12	1.68	0.59
4:S:177:MET:HE2	5:T:204:ARG:HG3	1.84	0.59
1:A:149:GLN:O	5:E:110:ARG:HD2	2.03	0.59
5:E:187:LYS:HB3	5:E:195:SER:OG	2.03	0.59
4:I:178:ARG:HB3	4:I:180:MET:HB2	1.84	0.59
5:J:21:LEU:HD12	5:J:89:LEU:HD23	1.85	0.59
1:P:81:LEU:HB3	1:P:118:TYR:CE2	2.38	0.59
1:P:176:ASN:HA	1:P:180:LEU:HD13	1.85	0.59
1:A:275:GLU:HB3	1:A:276:PRO:HD2	1.85	0.58
5:J:11:LEU:HD23	5:J:120:LEU:HD12	1.84	0.58
4:D:52:TYR:HB2	5:E:111:GLU:HG3	1.85	0.58
4:N:79:ALA:HB2	4:N:91:LEU:HD13	1.84	0.58
4:S:11:MET:HE2	4:S:11:MET:HA	1.84	0.58
1:F:15:PRO:HA	1:F:90:GLY:O	2.04	0.58
5:J:6:GLN:HE21	5:J:104:CYS:H	1.48	0.58
1:K:50:PRO:O	1:K:53:GLU:HG2	2.03	0.58
5:O:25:GLN:HB2	5:O:27:MET:HE2	1.84	0.58
2:B:13:HIS:HB2	2:B:21:ASN:ND2	2.19	0.58
4:D:158:ASN:O	4:D:159:VAL:HG22	2.03	0.58
1:P:45:TYR:CE2	1:P:67:ALA:HB2	2.38	0.58
5:T:139:PRO:HD3	5:T:152:LEU:HD12	1.86	0.58
4:S:25:HIS:NE2	4:S:39:ILE:HD12	2.19	0.58
4:D:206:ILE:HG13	4:D:207:ILE:N	2.11	0.58
1:K:5:MET:HB2	1:K:168:LEU:HD13	1.85	0.58
2:L:19:LYS:H	2:L:72:PRO:HD2	1.69	0.58
1:P:106:ASP:OD1	1:P:108:ARG:HG2	2.04	0.58
5:T:159:PHE:HE2	5:T:162:ASP:HA	1.68	0.58
1:F:195:SER:OG	1:F:198:GLU:HB2	2.04	0.58
5:J:189:GLN:O	5:J:195:SER:HB3	2.04	0.58
4:N:15:GLU:HA	4:N:94:VAL:HG23	1.85	0.58
4:D:128:GLN:HG2	4:D:183:LYS:HG3	1.84	0.58
1:K:263:HIS:CD2	1:K:265:GLY:H	2.22	0.58
4:D:21:LEU:HD12	4:D:89:LEU:HD23	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:39:MET:HB3	2:G:46:ILE:HD12	1.86	0.57
4:I:130:PRO:CG	4:I:154:ASP:HB2	2.33	0.57
4:I:158:ASN:H	4:I:158:ASN:HD22	1.52	0.57
4:N:95:SER:HB3	4:N:97:ARG:HD3	1.85	0.57
5:T:168:TRP:HD1	5:T:179:VAL:HG13	1.68	0.57
5:E:212:ASN:OD1	5:E:214:ARG:HB2	2.04	0.57
1:P:234:ARG:HD2	2:Q:10:TYR:CE1	2.39	0.57
4:I:188:VAL:HG23	5:J:202:ARG:HE	1.67	0.57
4:N:127:ILE:HG13	4:N:128:GLN:HG2	1.86	0.57
4:I:193:LYS:HD2	4:I:195:ASP:HB2	1.86	0.57
5:T:132:PRO:HA	5:T:159:PHE:HB3	1.86	0.57
5:T:143:GLU:CD	5:T:150:ALA:HB2	2.29	0.57
2:G:7:ILE:HG22	2:G:27:VAL:HG22	1.87	0.57
4:S:25:HIS:HE1	4:S:104:CYS:SG	2.27	0.57
1:F:204:TRP:HE3	1:F:206:LEU:HD11	1.69	0.57
2:G:52:SER:HB3	2:G:64:ILE:HG13	1.85	0.57
4:S:14:THR:H	4:S:17:GLU:CD	2.13	0.57
4:I:178:ARG:HB3	4:I:179:SER:HA	1.85	0.57
1:K:191:HIS:HA	1:K:201:LEU:HD12	1.85	0.57
4:N:4:THR:HG21	4:N:104:CYS:HB3	1.87	0.57
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.40	0.57
1:P:194:ARG:HG3	1:P:195:SER:H	1.70	0.57
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.40	0.56
4:D:26:ALA:HA	4:D:85:LYS:HA	1.87	0.56
4:D:150:PHE:HB3	4:D:153:PHE:HE1	1.67	0.56
1:P:8:PHE:HB3	2:Q:56:PHE:CE2	2.39	0.56
1:P:202:ARG:HB3	1:P:246:SER:HB3	1.87	0.56
5:T:149:LYS:CB	5:T:206:SER:HA	2.35	0.56
1:P:234:ARG:HD2	2:Q:10:TYR:CD1	2.41	0.56
5:E:21:LEU:HD22	5:E:118:THR:HG21	1.87	0.56
5:E:43:ARG:NH2	5:E:100:SER:HB2	2.18	0.56
4:I:209:GLU:CA	4:I:210:ASP:HB3	2.35	0.56
1:K:167:TRP:HB3	1:K:171:TYR:CE2	2.40	0.56
5:O:70:ASP:O	5:O:71:ILE:HD13	2.05	0.56
5:T:57:TYR:O	5:T:58:ASP:HB2	2.06	0.56
2:B:52:SER:HB3	2:B:65:LEU:H	1.71	0.56
5:E:131:PRO:HD3	5:E:239:PRO:HB3	1.88	0.56
5:J:43:ARG:HH21	5:J:100:SER:HB2	1.71	0.56
1:K:58:GLU:CD	1:K:58:GLU:H	2.14	0.56
1:A:8:PHE:HB3	2:B:56:PHE:CZ	2.41	0.56
1:A:16:GLY:O	1:A:18:GLU:HG3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:6:GLN:HE22	5:J:103:PHE:HA	1.70	0.56
5:J:95:LYS:HB2	5:J:98:GLN:HG3	1.88	0.56
2:G:11:SER:HB2	2:G:21:ASN:ND2	2.21	0.55
4:I:210:ASP:CB	4:I:211:THR:HG23	2.36	0.55
5:J:56:SER:HB2	5:J:87:PHE:CZ	2.41	0.55
2:L:11:SER:HB2	2:L:21:ASN:ND2	2.20	0.55
4:N:54:THR:HG23	4:N:81:LEU:HD23	1.88	0.55
1:F:14:ARG:HB3	1:F:17:LEU:HD13	1.88	0.55
5:T:243:ILE:N	5:T:243:ILE:HD13	2.22	0.55
1:A:260:ARG:HG2	1:A:271:THR:HG22	1.88	0.55
4:I:50:PRO:HG2	5:J:50:LEU:HD22	1.88	0.55
4:N:149:LEU:HD11	4:N:186:SER:HB2	1.89	0.55
4:D:20:HIS:HE1	4:I:20:HIS:CE1	2.23	0.55
1:P:47:PRO:HG3	1:P:60:TRP:CH2	2.42	0.55
4:D:206:ILE:O	4:D:207:ILE:HG12	2.06	0.55
4:N:95:SER:O	4:N:96:LEU:HB3	2.06	0.55
5:T:151:THR:HG22	5:T:152:LEU:H	1.72	0.55
1:K:103:LEU:HD11	1:K:165:VAL:HG13	1.89	0.55
3:C:3:LEU:HD12	3:C:4:GLU:H	1.72	0.54
4:N:66:ASN:O	4:N:67:THR:HB	2.08	0.54
1:A:5:MET:HE3	1:A:7:TYR:CE2	2.41	0.54
5:E:54:TYR:HA	5:E:68:GLU:O	2.07	0.54
1:F:251:LEU:HD12	1:F:254:GLU:OE1	2.08	0.54
1:K:232:GLU:HA	1:K:243:LYS:HZ2	1.72	0.54
1:A:13:SER:HB2	1:A:93:HIS:H	1.71	0.54
4:I:151:THR:HG22	4:I:186:SER:HB3	1.90	0.54
4:S:177:MET:HE2	5:T:204:ARG:CG	2.38	0.54
4:I:127:ILE:HD12	4:I:127:ILE:H	1.73	0.54
4:I:183:LYS:O	4:I:184:SER:HB3	2.08	0.54
4:D:30:GLY:HA2	4:D:84(C):ARG:HH12	1.72	0.54
4:I:39:ILE:HG13	4:I:39:ILE:O	2.08	0.54
4:N:19:VAL:HG23	4:N:94:VAL:CG1	2.37	0.54
5:J:40:TYR:HB2	5:J:105:ALA:HB3	1.90	0.54
1:K:219:LEU:HD13	1:K:257:TYR:CE2	2.42	0.54
2:L:49:VAL:HG22	2:L:68:THR:HB	1.89	0.54
1:P:13:SER:HA	1:P:20:PRO:HB3	1.90	0.54
5:T:2:MET:HE1	5:T:113:TYR:CZ	2.43	0.54
1:A:217:TRP:HB2	1:A:228:MET:HE2	1.90	0.54
2:G:39:MET:HE3	2:G:67:HIS:HA	1.90	0.54
1:K:211:ALA:HB1	1:K:233:THR:HG21	1.89	0.54
4:N:168:TYR:CD2	4:N:191:SER:HB3	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:72:GLN:HG3	1:P:75:ARG:NH2	2.23	0.54
4:S:96:LEU:HA	4:S:124:VAL:HG11	1.90	0.54
2:B:33:PRO:HG3	2:B:62:PHE:CZ	2.43	0.54
5:J:154:CYS:HB2	5:J:168:TRP:CH2	2.43	0.54
5:J:222:GLN:OE1	5:J:243:ILE:HG23	2.08	0.54
1:K:68:LYS:HE2	1:K:68:LYS:HA	1.90	0.54
1:K:188:HIS:CE1	1:K:204:TRP:HB2	2.42	0.54
1:K:218:GLN:HG2	1:K:223:GLU:HA	1.89	0.54
1:K:263:HIS:CD2	1:K:266:LEU:HD13	2.43	0.54
4:N:3:LYS:HB2	4:N:3:LYS:NZ	2.23	0.54
4:N:20:HIS:NE2	4:S:18:THR:HG21	2.23	0.53
4:S:193:LYS:HE2	4:S:195:ASP:HB3	1.89	0.53
5:T:58:ASP:O	5:T:59:VAL:C	2.50	0.53
5:T:168:TRP:CD1	5:T:179:VAL:HG13	2.43	0.53
1:A:213:ILE:HG12	1:A:214:THR:H	1.73	0.53
1:A:218:GLN:HG3	1:A:258:THR:HB	1.90	0.53
1:F:213:ILE:HD11	1:F:261:VAL:HG13	1.89	0.53
4:I:210:ASP:HB2	4:I:211:THR:HG23	1.90	0.53
1:P:47:PRO:HG3	1:P:60:TRP:CZ2	2.43	0.53
1:A:8:PHE:CD1	1:A:98:MET:HG2	2.43	0.53
1:F:35:ARG:HB3	1:F:48:ARG:HD3	1.90	0.53
4:I:46:PRO:O	4:I:47:LEU:HG	2.08	0.53
1:K:52:MET:C	1:K:54:GLN:H	2.17	0.53
1:K:185:PRO:HD2	1:K:266:LEU:HD11	1.88	0.53
1:F:14:ARG:HD2	1:F:17:LEU:HD22	1.90	0.53
2:Q:37:ILE:HB	2:Q:51:MET:HE1	1.90	0.53
1:K:96:GLN:OE1	2:L:31:HIS:HE1	1.92	0.53
4:N:58:GLN:O	4:N:59:GLN:C	2.51	0.53
4:I:149:LEU:HG	4:I:151:THR:HG23	1.91	0.53
5:O:95:LYS:HB2	5:O:98:GLN:HG3	1.91	0.53
4:S:18:THR:HA	4:S:92:PRO:O	2.08	0.53
1:F:234:ARG:HD2	2:G:10:TYR:CE1	2.43	0.53
4:I:151:THR:HG22	4:I:186:SER:CB	2.38	0.53
5:O:207:ALA:O	5:O:211:GLN:HG2	2.09	0.53
4:D:46:PRO:O	4:D:47:LEU:HB2	2.09	0.53
4:I:178:ARG:NH2	5:J:204:ARG:HD3	2.24	0.53
2:L:30:PHE:CE1	2:L:62:PHE:HB2	2.44	0.53
4:N:193:LYS:HD2	4:N:194:SER:N	2.24	0.53
1:A:217:TRP:CZ3	1:A:259:CYS:HB2	2.44	0.53
4:I:212:PHE:CE1	5:J:142:ALA:HB1	2.44	0.53
2:B:89:GLU:HB2	2:B:90:PRO:HD2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:77:ARG:HG3	5:E:90:ILE:HB	1.89	0.52
1:P:133:TRP:HB2	1:P:144:ARG:HG3	1.90	0.52
5:E:170:VAL:HG23	5:E:175:VAL:HG21	1.91	0.52
1:F:12:VAL:HG13	1:F:94:THR:HG23	1.92	0.52
4:I:134:VAL:HG12	4:I:211:THR:HG21	1.90	0.52
4:I:184:SER:HB2	5:J:204:ARG:HH21	1.73	0.52
1:P:8:PHE:HB3	2:Q:56:PHE:CZ	2.44	0.52
5:T:7:MET:HB3	5:T:8:PRO:CD	2.31	0.52
4:N:121:LEU:HD21	4:N:123:THR:HG23	1.91	0.52
4:N:191:SER:HB2	4:N:192:ASN:CG	2.34	0.52
5:O:58:ASP:O	5:O:80:ARG:HG2	2.10	0.52
5:T:23:CYS:HB2	5:T:41:TRP:CZ2	2.45	0.52
4:N:172:LYS:HA	4:N:187:ALA:HB2	1.91	0.52
1:P:51:TRP:O	1:P:54:GLN:HG2	2.09	0.52
4:N:105:ILE:HD13	4:N:114:LEU:HD13	1.92	0.52
5:T:68:GLU:HB3	5:T:72:PRO:CG	2.39	0.52
1:A:162:GLY:O	1:A:166:GLU:HG2	2.09	0.52
4:I:206:ILE:O	4:I:207:ILE:C	2.52	0.52
5:O:126:LEU:HD12	5:O:126:LEU:H	1.74	0.52
4:S:156:GLN:HE22	4:S:158:ASN:CG	2.18	0.52
5:T:232:TRP:HB2	5:T:238:LYS:HE2	1.92	0.52
4:D:170:THR:HG23	4:D:188:VAL:H	1.75	0.52
5:O:2:MET:HE2	5:O:113:TYR:CE1	2.44	0.52
5:O:24:GLY:HA2	5:O:85:GLU:O	2.09	0.52
5:T:25:GLN:HE22	5:T:29:HIS:H	1.55	0.52
5:J:136:VAL:HG23	5:J:246:ALA:HB3	1.92	0.52
4:N:43:ARG:HD2	4:N:53:VAL:HG22	1.92	0.52
4:N:54:THR:HB	4:N:69:ASN:OD1	2.09	0.52
4:N:90:ILE:O	4:N:91:LEU:HB2	2.09	0.52
4:S:45:VAL:HG22	4:S:100:ALA:HB2	1.90	0.52
5:J:238:LYS:HE3	5:J:240:VAL:CG2	2.40	0.52
5:O:208:THR:HA	5:O:211:GLN:HG2	1.91	0.52
4:D:128:GLN:HG2	4:D:183:LYS:CG	2.40	0.51
1:F:202:ARG:NH2	2:G:99:MET:HE2	2.24	0.51
1:P:5:MET:HE2	1:P:7:TYR:HE2	1.75	0.51
5:T:6:GLN:HE22	5:T:103:PHE:HA	1.75	0.51
4:I:209:GLU:HA	4:I:210:ASP:O	2.09	0.51
4:N:67:THR:OG1	4:S:68:THR:HG21	2.10	0.51
2:Q:95:TRP:CD1	2:Q:96:ASP:N	2.77	0.51
5:T:19:VAL:HG13	5:T:91:LEU:CD1	2.39	0.51
5:T:146:HIS:C	5:T:148:GLN:H	2.18	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:147:THR:O	5:T:149:LYS:HG2	2.10	0.51
1:A:81:LEU:HB3	1:A:118:TYR:CE2	2.46	0.51
4:D:158:ASN:C	4:D:160:SER:H	2.18	0.51
4:D:201:ALA:O	4:D:202:PHE:HB3	2.11	0.51
5:E:186:LEU:HD23	5:E:186:LEU:H	1.75	0.51
4:I:207:ILE:HG23	4:I:207:ILE:O	2.10	0.51
1:K:208:PHE:HE2	1:K:242:GLN:HA	1.76	0.51
5:O:187:LYS:O	5:O:190:PRO:HD3	2.10	0.51
2:G:24:ASN:ND2	2:G:65:LEU:HD11	2.25	0.51
2:G:33:PRO:HG3	2:G:62:PHE:CZ	2.45	0.51
5:O:66:ASN:HD22	5:O:78:VAL:CG2	2.18	0.51
4:S:46:PRO:O	4:S:47:LEU:HB2	2.10	0.51
1:A:208:PHE:CE2	1:A:242:GLN:HA	2.46	0.51
2:L:33:PRO:HG3	2:L:62:PHE:CE1	2.46	0.51
4:D:42:TYR:HD1	4:D:105:ILE:HD13	1.74	0.51
2:Q:36:GLU:HB3	2:Q:83:LYS:HB3	1.93	0.51
4:D:208:PRO:C	4:D:210:ASP:H	2.19	0.51
5:J:184:GLN:OE1	5:J:185:PRO:HD2	2.11	0.51
1:P:6:ARG:CG	1:P:6:ARG:NH1	2.61	0.51
4:S:135:TYR:CE1	5:T:143:GLU:HG2	2.46	0.51
4:S:175:LEU:O	4:S:176:ASP:HB2	2.11	0.51
2:B:2:GLN:HG2	2:B:32:PRO:HD3	1.91	0.51
5:E:132:PRO:HB3	5:E:159:PHE:CD1	2.46	0.51
1:K:31:LYS:HD2	1:K:209:TYR:OH	2.11	0.51
2:L:40:LEU:HD21	2:L:81:ARG:NH2	2.26	0.51
1:P:263:HIS:CD2	1:P:265:GLY:H	2.28	0.51
5:E:99:THR:OG1	5:E:121:THR:HA	2.11	0.50
4:I:133:ALA:CA	4:I:211:THR:HG22	2.41	0.50
5:O:21:LEU:HD22	5:O:118:THR:HG21	1.92	0.50
5:O:71:ILE:N	5:O:72:PRO:HD3	2.26	0.50
4:N:113:LYS:HE3	5:O:57:TYR:OH	2.11	0.50
3:C:7:ARG:HD2	5:E:109:GLY:O	2.11	0.50
4:D:68:THR:HG21	4:I:68:THR:CB	2.41	0.50
4:D:112:TYR:CE1	5:E:31:THR:HG21	2.47	0.50
5:J:71:ILE:N	5:J:72:PRO:HD3	2.26	0.50
2:L:56:PHE:HB2	2:L:61:SER:O	2.11	0.50
4:N:193:LYS:HD2	4:N:194:SER:HB3	1.94	0.50
1:A:182:THR:HB	1:A:209:TYR:O	2.11	0.50
4:D:4:THR:O	4:D:5:THR:HG23	2.12	0.50
4:D:14:THR:HG22	4:D:125:THR:HB	1.94	0.50
4:D:159:VAL:O	4:D:160:SER:C	2.54	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:27:VAL:HG12	2:Q:30:PHE:CD2	2.47	0.50
5:T:153:VAL:HG22	5:T:202:ARG:HB3	1.94	0.50
2:B:51:MET:HB3	2:B:64:ILE:HD11	1.93	0.50
2:G:33:PRO:HG3	2:G:62:PHE:CE1	2.46	0.50
4:D:141:LYS:HE3	4:D:141:LYS:HA	1.94	0.50
1:K:117:ALA:HB2	2:L:60:TRP:CE2	2.47	0.50
1:K:163:GLU:O	1:K:167:TRP:HD1	1.94	0.50
5:O:55:ILE:HD13	5:O:56:SER:N	2.26	0.50
1:K:81:LEU:HD13	1:K:118:TYR:CD1	2.47	0.50
5:O:70:ASP:C	5:O:72:PRO:HD3	2.37	0.50
1:P:56:GLY:O	1:P:59:TYR:HB3	2.12	0.50
1:F:206:LEU:N	1:F:206:LEU:HD12	2.26	0.50
2:G:21:ASN:CG	2:G:22:ILE:H	2.20	0.50
4:I:206:ILE:HG23	4:I:208:PRO:HD3	1.94	0.50
5:J:80:ARG:HD2	5:J:86:HIS:O	2.11	0.50
1:P:205:ALA:C	1:P:206:LEU:HD12	2.36	0.50
4:S:178:ARG:HD3	4:S:178:ARG:C	2.36	0.50
2:B:7:ILE:HD12	2:B:91:LYS:HG2	1.93	0.49
5:J:226:LEU:O	5:J:240:VAL:HA	2.11	0.49
5:O:5:THR:O	5:O:23:CYS:HA	2.11	0.49
4:S:183:LYS:CA	4:S:184:SER:HB2	2.43	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CZ2	2.47	0.49
2:B:15:PRO:HG2	2:B:97:ARG:HB2	1.94	0.49
1:K:103:LEU:HD12	1:K:168:LEU:HD23	1.93	0.49
5:O:126:LEU:O	5:O:232:TRP:HZ3	1.95	0.49
1:F:109:LEU:HD13	1:F:161:GLU:HA	1.94	0.49
1:F:111:ARG:HD3	1:F:113:TYR:CZ	2.47	0.49
1:K:181:ARG:HB3	1:K:181:ARG:NH1	2.27	0.49
1:F:133:TRP:HB2	1:F:144:ARG:HG3	1.94	0.49
1:F:271:THR:C	1:F:272:LEU:HD12	2.37	0.49
4:N:186:SER:OG	5:O:202:ARG:HD2	2.13	0.49
4:I:210:ASP:OD1	4:I:211:THR:HG23	2.12	0.49
1:K:27:TYR:HD1	1:K:32:GLU:HA	1.77	0.49
4:N:153:PHE:H	4:N:154:ASP:HB2	1.77	0.49
5:O:154:CYS:HB2	5:O:168:TRP:CZ2	2.48	0.49
4:D:139:ASP:HA	5:E:137:PHE:HA	1.94	0.49
1:F:263:HIS:CG	1:F:264:GLU:N	2.79	0.49
2:B:28:THR:HG22	2:B:63:TYR:HB2	1.95	0.49
1:F:263:HIS:CD2	1:F:264:GLU:H	2.29	0.49
4:N:18:THR:HA	4:N:92:PRO:O	2.12	0.49
1:A:224:LEU:O	1:A:228:MET:HE3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:238:ASP:HB3	2:L:12:ARG:NH2	2.27	0.49
4:S:173:CYS:O	4:S:174:VAL:HB	2.12	0.49
5:T:59:VAL:HG12	5:T:60:ASP:N	2.27	0.49
5:T:95:LYS:HD2	5:T:95:LYS:N	2.28	0.49
4:D:114:LEU:HD12	4:D:114:LEU:O	2.13	0.49
5:J:126:LEU:HD13	5:J:226:LEU:HD11	1.94	0.49
5:J:132:PRO:HG2	5:J:244:VAL:HG21	1.95	0.49
5:E:226:LEU:HD23	5:E:230:ASP:HB3	1.95	0.48
4:I:52:TYR:CB	5:J:111:GLU:HG3	2.43	0.48
1:K:232:GLU:HA	1:K:243:LYS:NZ	2.28	0.48
4:N:20:HIS:CE1	4:S:18:THR:HG21	2.48	0.48
5:T:58:ASP:OD1	5:T:84:ARG:HD3	2.12	0.48
5:T:59:VAL:O	5:T:80:ARG:HB3	2.13	0.48
5:T:151:THR:HG22	5:T:152:LEU:HD22	1.95	0.48
1:A:41:GLU:O	1:A:43:PRO:HD3	2.13	0.48
1:F:44:ARG:NH2	1:F:61:GLU:HG2	2.28	0.48
1:K:81:LEU:HD21	3:M:10:VAL:HG11	1.95	0.48
4:N:149:LEU:HG	4:N:151:THR:HG23	1.94	0.48
4:D:134:VAL:HA	4:D:149:LEU:O	2.13	0.48
4:D:141:LYS:O	4:D:142:SER:C	2.57	0.48
2:G:32:PRO:HD2	2:G:85:ASP:OD1	2.14	0.48
5:T:25:GLN:NE2	5:T:29:HIS:N	2.58	0.48
5:T:58:ASP:OD1	5:T:59:VAL:HG23	2.13	0.48
5:T:166:LEU:HD23	5:T:167:SER:N	2.27	0.48
2:B:37:ILE:HG12	2:B:82:VAL:HG22	1.94	0.48
5:E:243:ILE:O	5:E:243:ILE:HG13	2.13	0.48
4:I:66:ASN:HD22	4:I:82:ALA:HA	1.78	0.48
1:K:209:TYR:C	1:K:209:TYR:CD2	2.91	0.48
1:P:117:ALA:HB2	2:Q:60:TRP:CE2	2.49	0.48
2:G:96:ASP:OD1	2:G:99:MET:HB2	2.14	0.48
5:J:13:LYS:HD3	5:J:19:VAL:HG22	1.95	0.48
1:K:213:ILE:HG12	1:K:214:THR:N	2.24	0.48
4:N:41:TRP:CE3	4:N:89:LEU:HD22	2.48	0.48
4:S:41:TRP:CE3	4:S:89:LEU:HD22	2.48	0.48
1:F:117:ALA:HB2	2:G:60:TRP:CZ2	2.48	0.48
5:E:58:ASP:O	5:E:59:VAL:C	2.56	0.48
1:F:111:ARG:HD3	1:F:113:TYR:OH	2.14	0.48
2:G:41:LYS:HD3	2:G:41:LYS:C	2.39	0.48
4:I:30:GLY:HA2	4:I:84(C):ARG:NH1	2.28	0.48
5:J:129:VAL:HG11	5:J:226:LEU:HD22	1.96	0.48
5:T:2:MET:HE2	5:T:2:MET:HB3	1.71	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:144:ILE:HD12	5:T:144:ILE:H	1.78	0.48
2:G:40:LEU:HD11	2:G:81:ARG:HB2	1.95	0.48
5:J:192:LEU:C	5:J:194:ASP:H	2.22	0.48
4:N:112:TYR:HB3	5:O:40:TYR:OH	2.13	0.48
4:N:191:SER:HB2	4:N:192:ASN:ND2	2.29	0.48
5:O:168:TRP:CZ3	5:O:219:CYS:HB3	2.48	0.48
2:Q:40:LEU:HA	2:Q:46:ILE:HG13	1.95	0.48
4:S:112:TYR:HB3	5:T:40:TYR:OH	2.14	0.48
5:T:99:THR:HG22	5:T:99:THR:O	2.14	0.48
4:I:210:ASP:HA	4:I:211:THR:HA	1.58	0.48
5:J:6:GLN:HE22	5:J:104:CYS:H	1.58	0.48
4:N:81:LEU:C	4:N:81:LEU:HD12	2.39	0.48
1:P:230:LEU:HD12	1:P:244:TRP:O	2.14	0.48
2:Q:41:LYS:HB3	2:Q:78:TYR:CE2	2.48	0.48
1:A:103:LEU:HD13	1:A:168:LEU:HD23	1.96	0.47
4:D:168:TYR:O	4:D:189:ALA:HA	2.14	0.47
4:D:202:PHE:CE2	4:D:207:ILE:HD11	2.49	0.47
4:I:105:ILE:HG21	4:I:114:LEU:HB2	1.95	0.47
1:K:209:TYR:C	1:K:209:TYR:HD2	2.22	0.47
4:N:130:PRO:C	4:N:132:PRO:HD3	2.39	0.47
5:O:25:GLN:NE2	5:O:29:HIS:N	2.61	0.47
5:J:44:GLN:HG3	5:J:49:GLY:C	2.39	0.47
1:K:200:THR:O	1:K:201:LEU:HD13	2.14	0.47
4:N:118:LYS:HD3	4:N:118:LYS:O	2.14	0.47
2:Q:70:PHE:CE2	2:Q:72:PRO:HG3	2.49	0.47
5:T:70:ASP:O	5:T:71:ILE:HD13	2.15	0.47
1:A:150:SER:HA	5:E:110:ARG:HG2	1.97	0.47
1:F:218:GLN:NE2	1:F:260:ARG:HH11	2.03	0.47
5:O:80:ARG:HD2	5:O:86:HIS:O	2.14	0.47
1:P:209:TYR:CD1	1:P:210:PRO:HA	2.49	0.47
4:D:112:TYR:HB3	5:E:40:TYR:OH	2.15	0.47
1:F:47:PRO:HG3	1:F:60:TRP:CZ2	2.49	0.47
2:G:58:LYS:HD2	2:G:58:LYS:N	2.29	0.47
4:I:112:TYR:HB3	5:J:40:TYR:OH	2.14	0.47
5:J:6:GLN:NE2	5:J:104:CYS:N	2.52	0.47
1:K:33:PHE:CD2	1:K:34:VAL:HG13	2.49	0.47
5:T:3:LYS:N	5:T:27:MET:HE1	2.28	0.47
2:G:10:TYR:O	2:G:23:LEU:HD12	2.14	0.47
5:J:59:VAL:CG1	5:J:60:ASP:H	2.13	0.47
1:K:36:PHE:HB2	1:K:45:TYR:CE1	2.49	0.47
5:O:6:GLN:HE22	5:O:104:CYS:H	1.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:137:LEU:HD12	5:T:138:GLU:O	2.14	0.47
1:P:191:HIS:NE2	1:P:199:VAL:HG11	2.29	0.47
4:S:53:VAL:HG23	4:S:54:THR:N	2.28	0.47
5:T:2:MET:HA	5:T:27:MET:HE1	1.96	0.47
5:T:18:ASN:OD1	5:T:92:ASP:HA	2.14	0.47
2:B:28:THR:HG22	2:B:63:TYR:CB	2.45	0.47
4:I:46:PRO:HB2	4:I:47:LEU:HD23	1.97	0.47
4:I:78:MET:O	4:I:79:ALA:CB	2.62	0.47
4:I:127:ILE:O	4:I:128:GLN:C	2.57	0.47
5:J:4:VAL:O	5:J:116:PRO:HD3	2.13	0.47
5:O:154:CYS:HB2	5:O:168:TRP:CH2	2.49	0.47
1:P:202:ARG:HA	1:P:245:ALA:O	2.15	0.47
5:T:91:LEU:O	5:T:91:LEU:HD12	2.15	0.47
5:T:151:THR:HG22	5:T:152:LEU:N	2.30	0.47
1:F:123:TYR:CZ	1:F:140:ALA:HA	2.49	0.47
4:I:209:GLU:CA	4:I:210:ASP:CB	2.92	0.47
5:O:2:MET:HE2	5:O:113:TYR:CG	2.50	0.47
5:E:12:ILE:HD11	5:E:123:LEU:HD12	1.97	0.47
4:I:197:ALA:O	4:I:201:ALA:HB3	2.14	0.47
4:N:3:LYS:HG3	4:N:4:THR:H	1.79	0.47
4:S:137:LEU:N	4:S:137:LEU:HD22	2.30	0.47
4:S:150:PHE:HB2	4:S:187:ALA:HB3	1.97	0.47
5:T:132:PRO:O	5:T:133:GLU:C	2.57	0.47
1:F:255:GLN:CD	1:F:255:GLN:H	2.22	0.47
4:I:92:PRO:O	4:I:93:HIS:C	2.56	0.47
5:J:129:VAL:HG11	5:J:226:LEU:CD2	2.45	0.47
4:N:66:ASN:CG	4:N:67:THR:N	2.72	0.47
4:S:20:HIS:CD2	4:S:90:ILE:HG13	2.50	0.47
4:S:32:GLU:HG2	4:S:106:LEU:HB3	1.97	0.47
1:A:35:ARG:HB3	1:A:48:ARG:HD3	1.97	0.46
1:A:72:GLN:HG3	1:A:75:ARG:NH2	2.30	0.46
1:A:178:THR:C	1:A:180:LEU:H	2.23	0.46
2:G:79:ALA:HB2	2:G:94:TYR:CD2	2.50	0.46
5:J:223:PHE:CD1	5:J:224:TYR:N	2.83	0.46
4:N:105:ILE:HG21	4:N:114:LEU:HD13	1.96	0.46
5:O:23:CYS:O	5:O:86:HIS:HA	2.15	0.46
5:T:14:ARG:O	5:T:17:GLU:HB2	2.15	0.46
4:D:137:LEU:HB3	5:E:138:GLU:O	2.15	0.46
1:F:213:ILE:HG13	1:F:262:TYR:O	2.15	0.46
4:I:137:LEU:HD23	5:J:139:PRO:HA	1.98	0.46
4:S:39:ILE:HD11	4:S:41:TRP:HE1	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HD13	1:A:161:GLU:HA	1.97	0.46
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.97	0.46
2:B:14:PRO:HA	2:B:15:PRO:HD3	1.81	0.46
4:I:4:THR:HG22	4:I:25:HIS:HB3	1.97	0.46
4:I:28:ILE:HG13	4:I:32:GLU:HG3	1.96	0.46
4:I:178:ARG:HH21	5:J:204:ARG:HD3	1.79	0.46
1:K:35:ARG:CZ	2:L:53:ASP:HB3	2.46	0.46
4:N:67:THR:OG1	4:N:68:THR:N	2.48	0.46
4:N:95:SER:CB	4:N:97:ARG:HD3	2.46	0.46
5:T:159:PHE:CE2	5:T:162:ASP:HA	2.50	0.46
1:A:154:GLU:HB3	4:D:57:LEU:HD22	1.96	0.46
4:I:16:GLY:O	4:I:93:HIS:HA	2.14	0.46
5:J:139:PRO:HD3	5:J:152:LEU:HG	1.96	0.46
1:P:258:THR:HG22	1:P:273:ARG:HG2	1.97	0.46
2:Q:31:HIS:CD2	2:Q:32:PRO:HA	2.51	0.46
4:D:149:LEU:HG	4:D:151:THR:HG23	1.97	0.46
4:I:139:ASP:HA	5:J:137:PHE:HA	1.98	0.46
4:N:173:CYS:HB3	5:O:202:ARG:NH1	2.31	0.46
4:N:188:VAL:HG12	4:N:189:ALA:N	2.30	0.46
1:P:143:THR:HG21	3:R:10:VAL:HG13	1.97	0.46
4:S:124:VAL:O	4:S:124:VAL:HG13	2.14	0.46
5:E:27:MET:HE2	5:E:27:MET:HB3	1.80	0.46
4:I:128:GLN:NE2	4:I:182:PHE:HD1	2.13	0.46
4:N:96:LEU:HA	4:N:124:VAL:HG11	1.98	0.46
4:N:153:PHE:H	4:N:154:ASP:CB	2.28	0.46
5:O:243:ILE:HD12	5:O:243:ILE:O	2.15	0.46
1:A:209:TYR:CD2	1:A:209:TYR:C	2.94	0.46
1:A:234:ARG:HD2	1:A:242:GLN:OE1	2.16	0.46
5:J:25:GLN:NE2	5:J:29:HIS:N	2.62	0.46
4:N:50:PRO:HG3	5:O:50:LEU:CD1	2.40	0.46
5:O:41:TRP:CE2	5:O:89:LEU:HB2	2.51	0.46
5:O:130:PHE:CB	5:O:196:ARG:HH11	2.29	0.46
1:P:202:ARG:O	1:P:204:TRP:HD1	1.99	0.46
1:P:234:ARG:HD3	2:Q:8:GLN:NE2	2.30	0.46
4:S:11:MET:HE2	4:S:12:GLU:H	1.81	0.46
5:T:76:TYR:CE1	5:T:91:LEU:HD23	2.50	0.46
4:D:41:TRP:CG	4:D:89:LEU:HD13	2.50	0.46
4:I:209:GLU:HA	4:I:210:ASP:CB	2.45	0.46
1:K:17:LEU:O	1:K:19:GLU:N	2.49	0.46
5:E:96:THR:O	5:E:99:THR:HG22	2.16	0.46
5:E:223:PHE:O	5:E:241:THR:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:GLY:O	1:F:178:THR:HG22	2.16	0.46
1:F:202:ARG:HA	1:F:245:ALA:O	2.16	0.46
4:I:114:LEU:HD12	4:I:114:LEU:O	2.16	0.46
1:K:234:ARG:HB3	2:L:10:TYR:CZ	2.51	0.46
3:R:3:LEU:HD12	3:R:4:GLU:H	1.80	0.46
5:T:25:GLN:O	5:T:27:MET:HE3	2.16	0.46
5:E:99:THR:HG23	5:E:99:THR:O	2.16	0.45
1:F:190:THR:CG2	1:F:202:ARG:HB2	2.46	0.45
1:K:194:ARG:HD2	1:K:194:ARG:C	2.41	0.45
2:L:4:THR:HG23	2:L:5:PRO:HD2	1.97	0.45
1:P:81:LEU:HD13	1:P:118:TYR:CD2	2.51	0.45
4:I:4:THR:CG2	4:I:106:LEU:HG	2.46	0.45
4:I:155:SER:C	4:I:157:THR:H	2.23	0.45
5:O:10:TYR:HE1	5:O:119:ARG:HE	1.63	0.45
5:T:3:LYS:H	5:T:27:MET:HE1	1.81	0.45
5:E:133:GLU:O	5:E:157:THR:HG23	2.17	0.45
1:F:213:ILE:HG12	1:F:214:THR:N	2.32	0.45
5:J:125:ASP:C	5:J:127:LYS:H	2.25	0.45
4:N:193:LYS:HE2	4:N:193:LYS:HB3	1.78	0.45
5:O:25:GLN:O	5:O:26:ASP:HB2	2.17	0.45
4:S:180:MET:O	4:S:181:ASP:HB2	2.17	0.45
1:A:5:MET:CE	1:A:7:TYR:HE2	2.29	0.45
4:I:27:THR:HG22	4:I:27:THR:O	2.16	0.45
5:J:151:THR:HG22	5:J:204:ARG:HG3	1.99	0.45
1:K:185:PRO:HD2	1:K:266:LEU:CD1	2.46	0.45
1:P:28:VAL:HG23	1:P:33:PHE:CE1	2.51	0.45
1:A:70:GLN:HE22	3:C:5:ASN:HB2	1.81	0.45
5:E:7:MET:O	5:E:8:PRO:C	2.57	0.45
1:F:8:PHE:CE1	1:F:98:MET:HE3	2.52	0.45
1:F:211:ALA:HB1	1:F:233:THR:HG21	1.99	0.45
2:G:41:LYS:HB2	2:G:46:ILE:HD11	1.99	0.45
4:N:3:LYS:CG	4:N:4:THR:N	2.79	0.45
1:A:49:ALA:HB1	1:A:50:PRO:HD2	1.98	0.45
4:D:128:GLN:HG2	4:D:183:LYS:CD	2.47	0.45
4:S:91:LEU:HA	4:S:92:PRO:HD2	1.70	0.45
1:F:61:GLU:HA	1:F:64:THR:HG22	1.97	0.45
2:G:11:SER:HB2	2:G:21:ASN:HD22	1.82	0.45
5:J:48:LEU:HD12	5:J:48:LEU:N	2.31	0.45
5:J:66:ASN:HD22	5:J:78:VAL:HG23	1.82	0.45
5:J:214:ARG:CZ	5:J:214:ARG:HA	2.47	0.45
5:O:126:LEU:HD12	5:O:126:LEU:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:33:PHE:HD2	1:P:52:MET:HG3	1.81	0.45
4:S:6:GLN:OE1	4:S:104:CYS:HB3	2.17	0.45
5:T:59:VAL:HG13	5:T:81:LYS:O	2.17	0.45
5:J:186:LEU:C	5:J:186:LEU:HD12	2.42	0.45
1:K:49:ALA:HB1	1:K:50:PRO:HD2	1.98	0.45
1:K:223:GLU:H	1:K:223:GLU:HG2	1.45	0.45
1:P:45:TYR:HE2	1:P:67:ALA:HB2	1.79	0.45
5:T:27:MET:HG3	5:T:29:HIS:CD2	2.52	0.45
5:T:141:GLU:HA	5:T:144:ILE:HD13	1.99	0.45
4:D:183:LYS:HG2	4:D:184:SER:N	2.32	0.45
4:I:156:GLN:O	4:I:157:THR:HG22	2.17	0.45
1:K:44:ARG:O	1:K:46:GLU:HG3	2.17	0.45
4:N:198:CYS:O	4:N:199:ALA:HB3	2.17	0.45
4:D:206:ILE:HG23	4:D:207:ILE:CG2	2.47	0.45
1:F:274:TRP:CG	1:F:275:GLU:N	2.85	0.45
1:K:234:ARG:HB3	2:L:10:TYR:OH	2.17	0.45
1:A:109:LEU:CD1	1:A:161:GLU:HA	2.47	0.44
1:A:211:ALA:HB1	1:A:233:THR:HG21	1.98	0.44
5:E:134:VAL:HG21	5:E:221:VAL:CG1	2.47	0.44
4:I:96:LEU:C	4:I:98:ASP:H	2.25	0.44
1:P:33:PHE:CD2	1:P:34:VAL:HG13	2.52	0.44
4:S:156:GLN:HE22	4:S:158:ASN:ND2	2.16	0.44
4:D:80:PHE:HB3	4:I:80:PHE:CD1	2.52	0.44
1:F:12:VAL:HG22	1:F:94:THR:HG22	2.00	0.44
1:K:192:HIS:HA	1:K:193:PRO:HD3	1.78	0.44
4:N:137:LEU:HD12	4:N:137:LEU:N	2.32	0.44
5:O:140:SER:C	5:O:142:ALA:H	2.25	0.44
1:P:218:GLN:HE22	1:P:260:ARG:HH11	1.65	0.44
4:S:190:TRP:CE2	5:T:155:LEU:HD21	2.52	0.44
5:T:85:GLU:N	5:T:85:GLU:OE1	2.50	0.44
5:T:172:GLY:C	5:T:173:LYS:HD2	2.42	0.44
1:A:109:LEU:HD23	1:A:109:LEU:C	2.42	0.44
5:E:25:GLN:NE2	5:E:29:HIS:N	2.65	0.44
5:E:57:TYR:O	5:E:58:ASP:HB2	2.18	0.44
1:F:190:THR:HG22	1:F:202:ARG:HB2	1.99	0.44
5:J:59:VAL:O	5:J:80:ARG:HB3	2.17	0.44
2:L:81:ARG:HD3	2:L:92:THR:OG1	2.17	0.44
5:O:43:ARG:HB3	5:O:53:ILE:HD11	1.98	0.44
5:O:136:VAL:HG23	5:O:246:ALA:CB	2.45	0.44
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.52	0.44
5:E:136:VAL:HG23	5:E:246:ALA:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:129:ASN:HA	4:I:130:PRO:HD3	1.72	0.44
2:L:37:ILE:HG12	2:L:82:VAL:HG12	1.99	0.44
5:T:43:ARG:HB3	5:T:53:ILE:HD11	1.98	0.44
1:A:56:GLY:O	1:A:59:TYR:HB3	2.18	0.44
4:I:52:TYR:HB2	5:J:111:GLU:HG3	1.99	0.44
4:I:113:LYS:HE3	5:J:57:TYR:OH	2.18	0.44
5:T:181:THR:HG23	5:T:201:SER:HB2	1.99	0.44
1:F:199:VAL:O	1:F:249:VAL:HG22	2.18	0.44
4:N:201:ALA:O	4:N:202:PHE:HB3	2.18	0.44
1:A:185:PRO:HD3	1:A:263:HIS:CD2	2.53	0.44
1:A:234:ARG:HD3	2:B:10:TYR:CE1	2.52	0.44
4:D:168:TYR:HD2	4:D:190:TRP:CE2	2.35	0.44
5:J:126:LEU:O	5:J:232:TRP:HZ3	2.00	0.44
5:J:239:PRO:HB2	5:J:240:VAL:H	1.67	0.44
4:N:153:PHE:N	4:N:154:ASP:CA	2.77	0.44
4:I:147:VAL:HG21	4:I:188:VAL:HG13	1.99	0.44
4:I:179:SER:CA	4:I:180:MET:HB2	2.46	0.44
5:J:218:ARG:HG2	5:J:245:SER:OG	2.17	0.44
1:K:8:PHE:HB3	2:L:56:PHE:CE2	2.52	0.44
4:N:92:PRO:HB3	4:S:66:ASN:HD21	1.82	0.44
4:N:153:PHE:HB3	4:N:157:THR:O	2.18	0.44
1:P:194:ARG:HG3	1:P:195:SER:N	2.32	0.44
5:T:21:LEU:HD22	5:T:118:THR:HG21	2.00	0.44
2:B:95:TRP:CD1	2:B:96:ASP:H	2.36	0.44
4:D:167:VAL:HG11	4:D:200:ASN:HB3	2.00	0.44
4:N:52:TYR:CD2	5:O:111:GLU:HB3	2.53	0.44
4:S:173:CYS:HB2	5:T:202:ARG:NH1	2.24	0.44
5:T:41:TRP:HD1	5:T:87:PHE:CE2	2.36	0.44
1:A:94:THR:O	1:A:118:TYR:HD1	2.01	0.43
1:F:159:TYR:CG	3:H:3:LEU:HD13	2.53	0.43
4:I:41:TRP:CE3	4:I:89:LEU:HD13	2.53	0.43
1:K:36:PHE:HB2	1:K:45:TYR:CD1	2.53	0.43
1:K:201:LEU:N	1:K:201:LEU:HD22	2.33	0.43
5:T:223:PHE:O	5:T:241:THR:HA	2.18	0.43
1:A:15:PRO:HD3	1:A:92:SER:OG	2.19	0.43
4:D:206:ILE:CG1	4:D:207:ILE:N	2.76	0.43
5:E:7:MET:CB	5:E:8:PRO:CD	2.94	0.43
1:F:5:MET:O	1:F:100:GLY:HA3	2.18	0.43
4:S:84(C):ARG:O	4:S:85:LYS:HB2	2.18	0.43
4:S:90:ILE:HD12	4:S:90:ILE:N	2.33	0.43
1:A:215:LEU:HD22	1:A:261:VAL:HG22	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:29:SER:C	4:D:31:ASN:N	2.76	0.43
5:E:44:GLN:O	5:E:44:GLN:HG3	2.17	0.43
5:E:141:GLU:O	5:E:144:ILE:HG12	2.18	0.43
4:I:154:ASP:C	4:I:156:GLN:H	2.27	0.43
1:K:263:HIS:HD2	1:K:266:LEU:HD13	1.81	0.43
4:N:141:LYS:HE2	4:N:141:LYS:HA	2.00	0.43
5:O:224:TYR:HA	5:O:241:THR:HG23	2.00	0.43
4:S:182:PHE:O	4:S:183:LYS:HB3	2.18	0.43
5:T:143:GLU:O	5:T:144:ILE:C	2.60	0.43
5:T:175:VAL:HG22	5:T:176:HIS:N	2.32	0.43
4:D:20:HIS:CE1	4:I:20:HIS:CE1	2.95	0.43
1:F:98:MET:HE1	2:G:58:LYS:HG3	2.00	0.43
2:G:28:THR:HG23	2:G:63:TYR:HB3	2.00	0.43
5:J:252:ALA:O	5:J:253:ASP:C	2.60	0.43
5:T:41:TRP:CD1	5:T:87:PHE:CE2	3.06	0.43
1:A:5:MET:O	1:A:100:GLY:HA3	2.17	0.43
4:D:30:GLY:HA2	4:D:84(C):ARG:NH1	2.32	0.43
2:G:29:GLN:HA	2:G:61:SER:CB	2.38	0.43
5:J:103:PHE:CE1	5:J:117:GLY:HA3	2.53	0.43
5:J:131:PRO:HA	5:J:223:PHE:CD2	2.53	0.43
2:B:37:ILE:HB	2:B:51:MET:HE1	2.00	0.43
5:E:25:GLN:O	5:E:27:MET:HE3	2.19	0.43
1:F:186:LYS:HD2	1:F:186:LYS:N	2.33	0.43
4:N:195:ASP:O	4:N:196:PHE:C	2.61	0.43
5:O:240:VAL:O	5:O:242:GLN:HG2	2.18	0.43
1:P:49:ALA:HB1	1:P:50:PRO:HD2	2.01	0.43
2:Q:31:HIS:HA	2:Q:32:PRO:C	2.44	0.43
5:T:7:MET:CB	5:T:8:PRO:CD	2.93	0.43
1:A:7:TYR:CE1	3:C:2:SER:HB3	2.53	0.43
5:E:240:VAL:O	5:E:242:GLN:HG2	2.19	0.43
2:G:14:PRO:HA	2:G:15:PRO:HD3	1.70	0.43
2:G:32:PRO:HB2	2:G:33:PRO:CD	2.48	0.43
1:K:3:HIS:HA	1:K:29:ASP:OD1	2.18	0.43
2:Q:7:ILE:HB	2:Q:93:VAL:HG21	2.01	0.43
4:D:39:ILE:O	4:D:39:ILE:HG13	2.18	0.43
4:D:91:LEU:O	4:D:92:PRO:O	2.36	0.43
4:I:134:VAL:HG13	4:I:134:VAL:O	2.18	0.43
4:I:176:ASP:CG	4:I:177:MET:N	2.72	0.43
5:J:237:ALA:O	5:J:238:LYS:C	2.62	0.43
4:N:3:LYS:CG	4:N:4:THR:H	2.31	0.43
5:O:80:ARG:HH21	5:O:84:ARG:HA	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:102:ASP:HB2	1:P:111:ARG:HB3	2.00	0.43
2:Q:28:THR:HG22	2:Q:63:TYR:HB2	2.01	0.43
5:T:243:ILE:HG12	5:T:243:ILE:O	2.19	0.43
1:A:66:LYS:NZ	3:C:1:SER:HB3	2.34	0.43
1:A:81:LEU:HD21	3:C:10:VAL:HG11	2.01	0.43
4:D:46:PRO:O	4:D:47:LEU:CB	2.67	0.43
1:F:147:TRP:HB3	1:F:152:ALA:HB3	2.01	0.43
1:F:208:PHE:HE2	1:F:242:GLN:HA	1.84	0.43
5:J:20:LEU:HD21	5:J:88:SER:HB3	1.99	0.43
1:P:54:GLN:O	1:P:55:GLU:C	2.61	0.43
5:T:48:LEU:N	5:T:48:LEU:HD22	2.34	0.43
1:A:14:ARG:HB3	1:A:17:LEU:HD12	2.01	0.43
4:D:170:THR:HG22	4:D:188:VAL:O	2.19	0.43
1:F:205:ALA:O	1:F:242:GLN:HA	2.19	0.43
5:J:25:GLN:HG3	5:J:26:ASP:N	2.34	0.43
1:P:208:PHE:CE1	1:P:241:PHE:HB2	2.53	0.43
1:A:209:TYR:C	1:A:209:TYR:HD2	2.26	0.42
2:G:21:ASN:CG	2:G:22:ILE:N	2.77	0.42
2:G:70:PHE:HD2	2:G:78:TYR:CZ	2.37	0.42
4:I:139:ASP:HB3	5:J:137:PHE:CE2	2.54	0.42
5:J:102:TYR:O	5:J:117:GLY:HA2	2.19	0.42
2:L:17:ASN:HA	2:L:72:PRO:HB2	2.01	0.42
1:P:58:GLU:H	1:P:58:GLU:HG3	1.59	0.42
5:J:12:ILE:HD11	5:J:129:VAL:HG21	2.01	0.42
5:J:132:PRO:HG2	5:J:244:VAL:CG2	2.49	0.42
1:K:180:LEU:HD13	1:K:180:LEU:H	1.85	0.42
1:P:5:MET:HB2	1:P:168:LEU:HD13	2.01	0.42
5:T:45:ASP:C	5:T:47:GLY:H	2.27	0.42
5:T:71:ILE:N	5:T:72:PRO:HD3	2.33	0.42
1:A:225:THR:HG21	1:P:107:TRP:CE3	2.54	0.42
4:D:175:LEU:HD12	4:D:175:LEU:O	2.19	0.42
5:E:44:GLN:HE21	5:E:44:GLN:HB2	1.61	0.42
5:E:136:VAL:HG23	5:E:246:ALA:CB	2.49	0.42
5:T:81:LYS:HD3	5:T:81:LYS:HA	1.77	0.42
5:T:91:LEU:HD22	5:T:98:GLN:NE2	2.33	0.42
4:D:175:LEU:HB3	5:E:180:CYS:CB	2.41	0.42
4:I:147:VAL:CG2	4:I:188:VAL:HG13	2.49	0.42
5:J:58:ASP:OD1	5:J:84:ARG:HD3	2.19	0.42
5:J:77:ARG:NE	5:J:90:ILE:HG21	2.34	0.42
2:Q:49:VAL:HG22	2:Q:68:THR:HB	2.01	0.42
4:S:158:ASN:O	4:S:159:VAL:HG23	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:151:THR:O	4:S:152:ASP:HB2	2.20	0.42
5:T:187:LYS:HD2	5:T:190:PRO:HA	2.02	0.42
5:T:212:ASN:HB3	5:T:215:ASN:HB2	2.01	0.42
1:A:194:ARG:O	1:A:195:SER:HB3	2.19	0.42
4:I:46:PRO:O	4:I:48:GLN:N	2.48	0.42
1:K:272:LEU:HD12	1:K:272:LEU:O	2.20	0.42
4:N:82:ALA:HB2	4:S:80:PHE:CE2	2.55	0.42
5:T:2:MET:HE1	5:T:113:TYR:CE1	2.55	0.42
5:T:192:LEU:HD12	5:T:192:LEU:N	2.35	0.42
1:A:44:ARG:HB2	1:A:64:THR:OG1	2.20	0.42
5:E:214:ARG:HA	5:E:214:ARG:NE	2.34	0.42
5:J:25:GLN:O	5:J:26:ASP:CB	2.68	0.42
5:J:77:ARG:NH2	5:J:90:ILE:HG21	2.34	0.42
5:J:205:VAL:HG11	5:J:209:PHE:CD2	2.54	0.42
1:K:117:ALA:HB2	2:L:60:TRP:CZ2	2.55	0.42
5:O:20:LEU:HD21	5:O:88:SER:HB3	2.02	0.42
1:P:109:LEU:HG	1:P:110:LEU:N	2.34	0.42
2:Q:5:PRO:HD3	2:Q:86:SER:OG	2.19	0.42
5:T:50:LEU:HD12	5:T:50:LEU:H	1.84	0.42
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.95	0.42
4:I:178:ARG:H	4:I:179:SER:CB	2.31	0.42
5:T:146:HIS:C	5:T:148:GLN:N	2.75	0.42
5:T:160:TYR:HA	5:T:161:PRO:HA	1.86	0.42
4:D:127:ILE:HB	4:D:128:GLN:H	1.58	0.42
5:E:97:ASN:C	5:E:99:THR:H	2.27	0.42
1:F:210:PRO:HD3	1:F:264:GLU:OE2	2.19	0.42
3:H:10:VAL:O	3:H:10:VAL:HG12	2.18	0.42
1:K:167:TRP:HB3	1:K:171:TYR:HE2	1.81	0.42
5:T:212:ASN:HD22	5:T:212:ASN:C	2.28	0.42
2:B:39:MET:HB3	2:B:46:ILE:HD12	2.02	0.42
2:B:85:ASP:OD1	2:B:85:ASP:N	2.53	0.42
1:F:13:SER:O	1:F:92:SER:HA	2.20	0.42
4:S:15:GLU:HB3	4:S:126:PRO:HA	2.01	0.42
5:T:20:LEU:HD11	5:T:88:SER:HB3	2.01	0.42
5:T:211:GLN:HA	5:T:211:GLN:HE21	1.85	0.42
1:A:45:TYR:HE2	1:A:67:ALA:HB2	1.85	0.41
4:D:158:ASN:C	4:D:160:SER:N	2.78	0.41
2:G:50:GLU:O	2:G:66:ALA:HA	2.20	0.41
2:L:7:ILE:HD11	2:L:82:VAL:CG2	2.50	0.41
4:N:95:SER:O	4:N:96:LEU:CB	2.67	0.41
1:F:61:GLU:O	1:F:65:GLN:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:30:GLU:HG3	5:J:84:ARG:HH21	1.84	0.41
1:K:51:TRP:H	1:K:51:TRP:CD1	2.37	0.41
1:K:250:PRO:HB2	1:K:253:LYS:HD2	2.01	0.41
4:N:39:ILE:O	4:N:55:HIS:HA	2.20	0.41
4:S:5:THR:HG23	4:S:24:SER:HB2	2.02	0.41
5:T:224:TYR:HA	5:T:241:THR:HG23	2.02	0.41
1:F:80:ASN:HA	1:P:86:ASN:ND2	2.35	0.41
1:F:201:LEU:O	1:F:246:SER:HA	2.21	0.41
4:I:137:LEU:HD12	4:I:137:LEU:N	2.35	0.41
2:L:89:GLU:HA	2:L:90:PRO:HD3	1.96	0.41
5:O:181:THR:HG23	5:O:201:SER:HB2	2.03	0.41
2:Q:14:PRO:HA	2:Q:15:PRO:HD3	1.77	0.41
4:S:14:THR:CG2	4:S:127:ILE:HG13	2.51	0.41
4:S:44:GLN:HE22	5:T:50:LEU:HD11	1.84	0.41
4:D:25:HIS:O	4:D:25:HIS:ND1	2.51	0.41
1:F:8:PHE:HB3	2:G:56:PHE:CZ	2.54	0.41
1:F:44:ARG:CZ	1:F:64:THR:HG21	2.51	0.41
1:F:74:PHE:HZ	1:F:97:GLN:HG2	1.85	0.41
2:G:41:LYS:N	2:G:46:ILE:HD11	2.35	0.41
4:I:194:SER:C	4:I:196:PHE:H	2.27	0.41
5:J:21:LEU:HB2	5:J:89:LEU:HB3	2.01	0.41
5:J:31:THR:HA	5:J:56:SER:O	2.20	0.41
5:J:44:GLN:HB2	5:J:50:LEU:HD12	2.01	0.41
5:O:148:GLN:C	5:O:207:ALA:HB2	2.45	0.41
5:T:125:ASP:OD1	5:T:127:LYS:HB2	2.20	0.41
5:T:151:THR:OG1	5:T:204:ARG:HD2	2.19	0.41
5:E:232:TRP:NE1	5:E:234:GLN:HB2	2.35	0.41
1:F:10:THR:O	1:F:22:TYR:HA	2.21	0.41
5:T:44:GLN:HB2	5:T:50:LEU:HG	2.02	0.41
4:D:91:LEU:HA	4:D:92:PRO:HD2	1.81	0.41
4:N:21:LEU:HA	4:N:22:PRO:HD3	1.98	0.41
1:P:226:GLN:O	1:P:227:ASP:C	2.63	0.41
4:D:207:ILE:C	4:D:209:GLU:H	2.28	0.41
4:I:127:ILE:H	4:I:127:ILE:CD1	2.30	0.41
4:I:149:LEU:HD12	4:I:150:PHE:H	1.85	0.41
1:K:258:THR:HG22	1:K:273:ARG:HD3	2.03	0.41
5:O:130:PHE:HA	5:O:131:PRO:HD3	1.87	0.41
5:O:163:HIS:HB3	5:O:224:TYR:HB2	2.02	0.41
3:R:10:VAL:OXT	3:R:10:VAL:HG12	2.20	0.41
5:T:143:GLU:CG	5:T:150:ALA:HB2	2.50	0.41
2:B:23:LEU:HB2	2:B:70:PHE:CD1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84(C):ARG:O	4:D:85:LYS:HB2	2.21	0.41
4:D:200:ASN:O	4:D:201:ALA:C	2.64	0.41
1:F:273:ARG:HB3	1:F:274:TRP:H	1.54	0.41
4:I:32:GLU:HB3	4:I:108:GLY:HA2	2.02	0.41
4:I:183:LYS:HD3	5:J:149:LYS:HZ2	1.85	0.41
2:L:16:GLU:HB2	2:L:19:LYS:HD2	2.02	0.41
4:N:28:ILE:HD11	4:N:32:GLU:HB2	2.03	0.41
5:O:61:SER:C	5:O:66:ASN:OD1	2.63	0.41
1:A:107:TRP:CE3	1:P:225:THR:HG22	2.56	0.41
1:A:202:ARG:HD3	1:A:244:TRP:CD2	2.55	0.41
1:A:225:THR:HB	1:P:107:TRP:CG	2.56	0.41
5:E:182:ASP:HB2	5:E:199:LEU:CD1	2.51	0.41
1:F:24:SER:HB3	1:F:36:PHE:HB3	2.03	0.41
1:F:81:LEU:HD13	1:F:118:TYR:CD1	2.56	0.41
4:I:183:LYS:O	4:I:184:SER:CB	2.69	0.41
5:J:181:THR:HG23	5:J:201:SER:HB2	2.01	0.41
1:K:181:ARG:HB3	1:K:181:ARG:CZ	2.51	0.41
1:K:192:HIS:HB2	1:K:200:THR:O	2.20	0.41
5:O:59:VAL:HG12	5:O:60:ASP:N	2.34	0.41
5:O:77:ARG:NH1	5:O:90:ILE:HD12	2.36	0.41
5:O:232:TRP:HH2	5:O:236:ARG:NH1	2.18	0.41
1:P:51:TRP:CD1	1:P:51:TRP:H	2.37	0.41
1:P:184:SER:HA	1:P:185:PRO:HD3	1.87	0.41
1:P:234:ARG:HG3	1:P:242:GLN:HG3	2.02	0.41
5:T:151:THR:HB	5:T:203:LEU:O	2.21	0.41
1:A:175:GLY:O	1:A:179:LEU:HG	2.21	0.41
1:A:219:LEU:HD13	1:A:257:TYR:CZ	2.56	0.41
5:J:39:MET:HA	5:J:105:ALA:O	2.21	0.41
1:K:8:PHE:HB3	2:L:56:PHE:CZ	2.56	0.41
1:K:78:LEU:O	1:K:82:LEU:HG	2.21	0.41
1:K:209:TYR:HD2	1:K:210:PRO:N	2.19	0.41
1:K:217:TRP:CE2	1:K:247:VAL:HG21	2.56	0.41
4:N:82:ALA:HB2	4:S:80:PHE:CZ	2.56	0.41
5:O:66:ASN:ND2	5:O:78:VAL:HG23	2.25	0.41
1:P:201:LEU:O	1:P:246:SER:HA	2.21	0.41
4:S:128:GLN:O	4:S:130:PRO:HD3	2.21	0.41
5:T:96:THR:HG21	5:T:124:GLU:HG3	2.03	0.41
5:T:187:LYS:HA	5:T:197:TYR:HA	2.03	0.41
1:A:25:VAL:HG12	1:A:27:TYR:CE1	2.56	0.40
1:A:38:SER:O	1:A:43:PRO:HG3	2.22	0.40
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:O	1:A:164:CYS:HB3	2.21	0.40
1:A:206:LEU:N	1:A:206:LEU:HD12	2.36	0.40
4:I:137:LEU:HB3	5:J:138:GLU:O	2.21	0.40
5:J:77:ARG:HE	5:J:90:ILE:HG21	1.85	0.40
1:K:259:CYS:O	1:K:271:THR:HG23	2.20	0.40
4:N:191:SER:HA	4:N:192:ASN:HA	1.73	0.40
1:P:169:HIS:O	1:P:173:LYS:HG3	2.20	0.40
4:S:83:ILE:N	4:S:83:ILE:HD12	2.37	0.40
2:B:7:ILE:HD11	2:B:82:VAL:HB	2.02	0.40
5:J:202:ARG:HD2	5:J:202:ARG:N	2.35	0.40
3:M:7:ARG:NH2	4:N:40:TYR:CE2	2.89	0.40
4:N:197:ALA:O	4:N:198:CYS:C	2.63	0.40
5:O:58:ASP:CG	5:O:59:VAL:H	2.28	0.40
1:P:72:GLN:HG3	1:P:75:ARG:HH22	1.87	0.40
3:C:10:VAL:O	3:C:10:VAL:CG1	2.64	0.40
4:D:207:ILE:HG13	4:D:209:GLU:N	2.17	0.40
5:E:71:ILE:N	5:E:72:PRO:HD3	2.33	0.40
5:J:17:GLU:HG2	5:J:18:ASN:H	1.86	0.40
4:N:20:HIS:HE1	4:S:18:THR:OG1	2.03	0.40
5:O:140:SER:C	5:O:142:ALA:N	2.80	0.40
2:Q:41:LYS:HB3	2:Q:78:TYR:CD2	2.56	0.40
5:T:45:ASP:C	5:T:47:GLY:N	2.79	0.40
1:A:147:TRP:HA	1:A:150:SER:OG	2.22	0.40
5:E:220:GLN:HE21	5:E:243:ILE:HB	1.87	0.40
5:J:56:SER:HB3	5:J:80:ARG:HH11	1.87	0.40
1:K:185:PRO:HA	1:K:207:GLY:O	2.21	0.40
4:N:83:ILE:HG13	4:N:84:ALA:O	2.21	0.40
5:O:79:SER:HB3	5:O:88:SER:HB2	2.02	0.40
5:T:1:ASP:N	5:T:3:LYS:HE3	2.37	0.40
5:T:192:LEU:HD12	5:T:192:LEU:H	1.85	0.40
1:A:106:ASP:C	1:A:108:ARG:H	2.29	0.40
2:B:22:ILE:HD13	2:B:69:GLU:HA	2.04	0.40
5:E:77:ARG:CZ	5:E:90:ILE:HG21	2.52	0.40
1:F:72:GLN:HE21	1:F:72:GLN:HB3	1.54	0.40
2:G:22:ILE:HD13	2:G:69:GLU:HA	2.04	0.40
2:L:71:THR:HA	2:L:72:PRO:HD3	1.85	0.40
1:P:62:ARG:O	1:P:66:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	273/275 (99%)	244 (89%)	26 (10%)	3 (1%)	11	43
1	F	263/275 (96%)	222 (84%)	39 (15%)	2 (1%)	16	50
1	K	273/275 (99%)	235 (86%)	30 (11%)	8 (3%)	3	24
1	P	271/275 (98%)	244 (90%)	25 (9%)	2 (1%)	18	52
2	B	96/99 (97%)	87 (91%)	7 (7%)	2 (2%)	5	31
2	G	96/99 (97%)	82 (85%)	11 (12%)	3 (3%)	3	22
2	L	96/99 (97%)	81 (84%)	13 (14%)	2 (2%)	5	31
2	Q	96/99 (97%)	87 (91%)	9 (9%)	0	100	100
3	C	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	1
3	H	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	M	8/10 (80%)	7 (88%)	0	1 (12%)	0	1
3	R	8/10 (80%)	7 (88%)	0	1 (12%)	0	1
4	D	183/195 (94%)	132 (72%)	37 (20%)	14 (8%)	1	5
4	I	184/195 (94%)	128 (70%)	45 (24%)	11 (6%)	1	10
4	N	170/195 (87%)	119 (70%)	40 (24%)	11 (6%)	1	8
4	S	168/195 (86%)	132 (79%)	31 (18%)	5 (3%)	3	23
5	E	238/240 (99%)	206 (87%)	24 (10%)	8 (3%)	3	20
5	J	238/240 (99%)	200 (84%)	30 (13%)	8 (3%)	3	20
5	O	238/240 (99%)	207 (87%)	25 (10%)	6 (2%)	4	27
5	T	238/240 (99%)	197 (83%)	34 (14%)	7 (3%)	3	24
All	All	3153/3276 (96%)	2629 (83%)	429 (14%)	95 (3%)	3	23

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	5	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	92	PRO
4	D	179	SER
5	E	8	PRO
5	E	68	GLU
4	I	208	PRO
5	J	68	GLU
5	J	239	PRO
2	L	17	ASN
4	N	67	THR
4	N	68	THR
4	N	179	SER
4	N	181	ASP
4	S	92	PRO
4	S	155	SER
5	T	8	PRO
5	T	59	VAL
5	T	252	ALA
4	D	15	GLU
4	D	159	VAL
5	E	48	LEU
5	E	59	VAL
5	E	158	GLY
4	I	93	HIS
4	I	182	PHE
5	J	48	LEU
5	J	240	VAL
1	K	18	GLU
1	K	255	GLN
4	N	59	GLN
4	N	92	PRO
4	N	194	SER
5	O	48	LEU
5	O	158	GLY
4	S	156	GLN
5	T	58	ASP
5	T	110	ARG
5	T	133	GLU
1	A	136	ALA
4	D	128	GLN
4	D	142	SER
4	D	158	ASN
4	D	193	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	58	ASP
5	E	110	ARG
1	F	263	HIS
4	I	47	LEU
4	I	128	GLN
4	I	184	SER
5	J	59	VAL
5	J	236	ARG
1	K	212	ASP
4	N	91	LEU
4	N	152	ASP
5	O	58	ASP
5	O	146	HIS
5	O	248	ALA
2	B	17	ASN
2	B	90	PRO
4	D	26	ALA
4	D	127	ILE
2	G	45	LYS
2	G	52	SER
2	G	88	ALA
4	I	79	ALA
4	I	199	ALA
5	J	7	MET
1	K	43	PRO
1	K	195	SER
3	M	5	ASN
1	P	195	SER
4	S	176	ASP
1	A	107	TRP
4	D	126	PRO
4	D	184	SER
4	I	46	PRO
4	I	210	ASP
1	K	226	GLN
2	L	48	LYS
4	N	126	PRO
1	P	269	PRO
4	S	174	VAL
1	A	41	GLU
4	D	134	VAL
4	I	23	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	J	146	HIS
3	R	5	ASN
4	D	206	ILE
5	E	47	GLY
1	F	43	PRO
4	N	127	ILE
5	O	59	VAL
5	T	144	ILE
1	K	267	PRO
1	K	269	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	234/234 (100%)	225 (96%)	9 (4%)	29	62
1	F	227/234 (97%)	221 (97%)	6 (3%)	40	69
1	K	234/234 (100%)	220 (94%)	14 (6%)	17	50
1	P	232/234 (99%)	223 (96%)	9 (4%)	28	62
2	B	93/94 (99%)	91 (98%)	2 (2%)	45	71
2	G	93/94 (99%)	87 (94%)	6 (6%)	15	47
2	L	93/94 (99%)	88 (95%)	5 (5%)	20	53
2	Q	93/94 (99%)	92 (99%)	1 (1%)	65	79
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
3	M	9/9 (100%)	9 (100%)	0	100	100
3	R	9/9 (100%)	9 (100%)	0	100	100
4	D	169/175 (97%)	157 (93%)	12 (7%)	13	44
4	I	168/175 (96%)	151 (90%)	17 (10%)	7	30
4	N	154/175 (88%)	139 (90%)	15 (10%)	8	32
4	S	154/175 (88%)	141 (92%)	13 (8%)	10	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	213/213 (100%)	199 (93%)	14 (7%)	15	47
5	J	213/213 (100%)	202 (95%)	11 (5%)	21	54
5	O	213/213 (100%)	204 (96%)	9 (4%)	26	60
5	T	213/213 (100%)	197 (92%)	16 (8%)	12	42
All	All	2832/2900 (98%)	2673 (94%)	159 (6%)	19	52

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	46	GLU
1	A	78	LEU
1	A	94	THR
1	A	145	ARG
1	A	179	LEU
1	A	181	ARG
1	A	209	TYR
1	A	247	VAL
2	B	61	SER
2	B	91	LYS
4	D	5	THR
4	D	11	MET
4	D	17	GLU
4	D	18	THR
4	D	39	ILE
4	D	115	THR
4	D	127	ILE
4	D	128	GLN
4	D	137	LEU
4	D	141	LYS
4	D	170	THR
4	D	207	ILE
5	E	7	MET
5	E	12	ILE
5	E	17	GLU
5	E	31	THR
5	E	44	GLN
5	E	68	GLU
5	E	84	ARG
5	E	96	THR
5	E	157	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	193	ASN
5	E	202	ARG
5	E	211	GLN
5	E	221	VAL
5	E	222	GLN
1	F	45	TYR
1	F	72	GLN
1	F	94	THR
1	F	179	LEU
1	F	230	LEU
1	F	255	GLN
2	G	28	THR
2	G	75	THR
2	G	81	ARG
2	G	85	ASP
2	G	92	THR
2	G	93	VAL
4	I	11	MET
4	I	18	THR
4	I	31	ASN
4	I	39	ILE
4	I	43	ARG
4	I	45	VAL
4	I	81	LEU
4	I	115	THR
4	I	127	ILE
4	I	128	GLN
4	I	147	VAL
4	I	157	THR
4	I	158	ASN
4	I	180	MET
4	I	182	PHE
4	I	210	ASP
4	I	211	THR
5	J	5	THR
5	J	12	ILE
5	J	27	MET
5	J	31	THR
5	J	51	GLN
5	J	85	GLU
5	J	95	LYS
5	J	120	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	J	199	LEU
5	J	230	ASP
5	J	243	ILE
1	K	17	LEU
1	K	45	TYR
1	K	58	GLU
1	K	61	GLU
1	K	106	ASP
1	K	119	GLU
1	K	141	GLN
1	K	149	GLN
1	K	180	LEU
1	K	201	LEU
1	K	209	TYR
1	K	217	TRP
1	K	223	GLU
1	K	226	GLN
2	L	2	GLN
2	L	8	GLN
2	L	38	GLN
2	L	70	PHE
2	L	91	LYS
4	N	3	LYS
4	N	12	GLU
4	N	18	THR
4	N	31	ASN
4	N	47	LEU
4	N	69	ASN
4	N	78	MET
4	N	83	ILE
4	N	93	HIS
4	N	97	ARG
4	N	115	THR
4	N	118	LYS
4	N	121	LEU
4	N	147	VAL
4	N	172	LYS
5	O	7	MET
5	O	27	MET
5	O	45	ASP
5	O	54	TYR
5	O	55	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	O	90	ILE
5	O	111	GLU
5	O	192	LEU
5	O	243	ILE
1	P	6	ARG
1	P	9	GLU
1	P	17	LEU
1	P	58	GLU
1	P	107	TRP
1	P	109	LEU
1	P	143	THR
1	P	145	ARG
1	P	270	LEU
2	Q	58	LYS
4	S	5	THR
4	S	11	MET
4	S	18	THR
4	S	39	ILE
4	S	68	THR
4	S	97	ARG
4	S	127	ILE
4	S	136	GLN
4	S	156	GLN
4	S	159	VAL
4	S	172	LYS
4	S	183	LYS
4	S	196	PHE
5	T	12	ILE
5	T	19	VAL
5	T	25	GLN
5	T	27	MET
5	T	54	TYR
5	T	84	ARG
5	T	90	ILE
5	T	91	LEU
5	T	95	LYS
5	T	146	HIS
5	T	152	LEU
5	T	193	ASN
5	T	202	ARG
5	T	211	GLN
5	T	212	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	T	243	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	87	GLN
1	A	96	GLN
1	A	127	ASN
1	A	169	HIS
1	A	192	HIS
1	A	226	GLN
1	A	263	HIS
2	B	2	GLN
2	B	31	HIS
4	D	20	HIS
4	D	44	GLN
4	D	136	GLN
4	D	185	ASN
4	D	192	ASN
4	D	204	ASN
5	E	18	ASN
5	E	29	HIS
5	E	44	GLN
5	E	112	GLN
5	E	146	HIS
5	E	193	ASN
5	E	216	HIS
1	F	42	ASN
1	F	65	GLN
1	F	72	GLN
1	F	87	GLN
1	F	97	GLN
1	F	127	ASN
1	F	149	GLN
1	F	169	HIS
1	F	174	ASN
1	F	255	GLN
2	G	67	HIS
4	I	20	HIS
4	I	58	GLN
4	I	66	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	I	93	HIS
4	I	103	HIS
4	I	111	ASN
4	I	128	GLN
4	I	158	ASN
5	J	6	GLN
5	J	18	ASN
5	J	29	HIS
5	J	112	GLN
5	J	146	HIS
5	J	171	ASN
5	J	176	HIS
5	J	216	HIS
5	J	242	GLN
1	K	3	HIS
1	K	87	GLN
1	K	188	HIS
1	K	263	HIS
2	L	2	GLN
2	L	8	GLN
2	L	31	HIS
4	N	20	HIS
4	N	25	HIS
4	N	59	GLN
4	N	66	ASN
4	N	103	HIS
4	N	128	GLN
4	N	136	GLN
5	O	6	GLN
5	O	29	HIS
5	O	51	GLN
5	O	97	ASN
5	O	112	GLN
5	O	216	HIS
5	O	222	GLN
5	O	242	GLN
1	P	54	GLN
1	P	65	GLN
1	P	87	GLN
1	P	96	GLN
1	P	127	ASN
1	P	141	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	169	HIS
1	P	176	ASN
1	P	256	ASN
1	P	263	HIS
2	Q	2	GLN
2	Q	8	GLN
2	Q	31	HIS
3	R	5	ASN
4	S	20	HIS
4	S	44	GLN
4	S	59	GLN
4	S	128	GLN
4	S	156	GLN
5	T	6	GLN
5	T	29	HIS
5	T	98	GLN
5	T	193	ASN
5	T	211	GLN
5	T	215	ASN
5	T	222	GLN
5	T	234	GLN
5	T	242	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 [i](#)

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, 95th 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	275/275 (100%)	0.19	2 (0%) 84 69	27, 74, 122, 148	1 (0%)
1	F	267/275 (97%)	0.47	11 (4%) 41 25	37, 100, 168, 201	1 (0%)
1	K	275/275 (100%)	0.48	12 (4%) 39 24	29, 94, 177, 194	0
1	P	273/275 (99%)	0.44	9 (3%) 49 30	38, 90, 152, 165	1 (0%)
2	B	98/99 (98%)	0.12	1 (1%) 79 63	42, 68, 103, 112	0
2	G	98/99 (98%)	0.53	1 (1%) 79 63	54, 104, 152, 156	0
2	L	98/99 (98%)	0.49	1 (1%) 79 63	53, 100, 144, 151	0
2	Q	98/99 (98%)	0.60	1 (1%) 79 63	58, 97, 129, 145	0
3	C	10/10 (100%)	-0.18	0 100 100	31, 38, 66, 70	0
3	H	10/10 (100%)	-0.12	0 100 100	40, 49, 81, 88	0
3	M	10/10 (100%)	-0.22	0 100 100	37, 44, 71, 83	0
3	R	10/10 (100%)	-0.09	0 100 100	42, 49, 80, 86	0
4	D	189/195 (96%)	0.66	13 (6%) 23 14	32, 79, 149, 169	0
4	I	188/195 (96%)	0.48	5 (2%) 56 36	40, 85, 146, 163	0
4	N	174/195 (89%)	0.62	12 (6%) 23 14	37, 79, 162, 179	0
4	S	174/195 (89%)	0.59	13 (7%) 20 13	40, 85, 150, 197	0
5	E	240/240 (100%)	0.13	0 100 100	32, 69, 120, 135	0
5	J	240/240 (100%)	0.19	2 (0%) 82 67	32, 69, 128, 152	0
5	O	240/240 (100%)	0.10	0 100 100	31, 69, 113, 149	0
5	T	240/240 (100%)	0.28	2 (0%) 82 67	40, 90, 135, 155	0
All	All	3207/3276 (97%)	0.37	85 (2%) 56 36	27, 82, 152, 201	3 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	205	ALA	4.3
4	N	68	THR	3.7
4	S	202	PHE	3.7
4	S	167	VAL	3.6
1	P	248	VAL	3.5
1	K	177	ALA	3.5
1	F	185	PRO	3.2
1	K	215	LEU	3.1
4	S	169	ILE	3.0
4	D	208	PRO	2.9
1	K	193	PRO	2.9
1	P	274	TRP	2.9
4	D	202	PHE	2.9
1	F	242	GLN	2.9
1	P	261	VAL	2.9
1	P	217	TRP	2.8
4	D	198	CYS	2.7
4	I	198	CYS	2.7
1	P	177	ALA	2.7
4	S	175	LEU	2.7
4	I	206	ILE	2.6
4	S	159	VAL	2.6
4	N	202	PHE	2.6
4	D	201	ALA	2.5
4	D	206	ILE	2.5
4	N	188	VAL	2.5
1	K	206	LEU	2.5
1	F	180	LEU	2.5
4	S	201	ALA	2.5
1	F	204	TRP	2.5
1	F	178	THR	2.4
1	F	200	THR	2.4
2	Q	14	PRO	2.4
1	P	201	LEU	2.4
1	P	272	LEU	2.4
1	P	249	VAL	2.4
5	T	172	GLY	2.4
4	N	79	ALA	2.4
4	N	182	PHE	2.4
1	K	104	GLY	2.4
4	S	182	PHE	2.4
1	P	179	LEU	2.3
4	S	27	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	78	MET	2.3
4	S	170	THR	2.3
1	K	261	VAL	2.3
2	L	15	PRO	2.3
4	D	213	PHE	2.3
1	F	261	VAL	2.3
1	K	247	VAL	2.3
5	J	26	ASP	2.3
5	J	71	ILE	2.2
1	K	189	VAL	2.2
4	S	127	ILE	2.2
1	K	2	PRO	2.2
4	S	78	MET	2.2
4	S	190	TRP	2.2
1	A	2	PRO	2.2
4	N	46	PRO	2.2
4	I	167	VAL	2.2
4	D	205	SER	2.2
5	T	150	ALA	2.2
4	D	153	PHE	2.1
4	D	185	ASN	2.1
4	D	207	ILE	2.1
1	K	236	ALA	2.1
4	N	201	ALA	2.1
4	D	140	SER	2.1
4	I	205	SER	2.1
1	F	256	ASN	2.1
1	F	201	LEU	2.1
2	B	85	ASP	2.1
4	N	152	ASP	2.1
2	G	54	MET	2.1
1	A	105	SER	2.1
4	N	184	SER	2.1
4	N	191	SER	2.1
1	K	270	LEU	2.1
4	N	67	THR	2.1
1	F	177	ALA	2.1
4	D	17	GLU	2.1
4	I	182	PHE	2.1
4	S	124	VAL	2.0
1	K	59	TYR	2.0
4	N	131	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.