



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:47 AM GMT

PDB ID : 3PQY
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

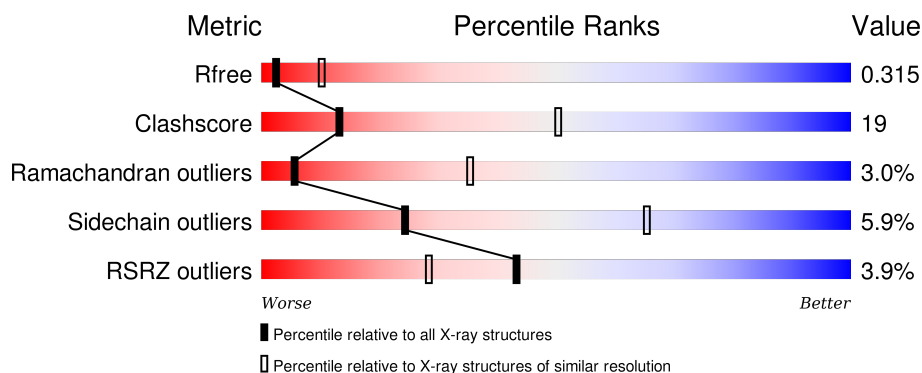
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div>3%</div> <div>61%</div> <div>36%</div> <div>.</div> </div>
1	F	275	<div> <div>8%</div> <div>63%</div> <div>33%</div> <div>..</div> </div>
1	K	275	<div> <div>9%</div> <div>64%</div> <div>33%</div> <div>.</div> </div>
1	P	275	<div> <div>7%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
2	B	99	<div> <div>64%</div> <div>32%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	99	
2	L	99	
2	Q	99	
3	C	10	
3	H	10	
3	M	10	
3	R	10	
4	D	195	
4	I	195	
4	N	195	
4	S	195	
5	E	240	
5	J	240	
5	O	240	
5	T	240	

2 Entry composition [i](#)

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			

- 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 alpha chain of the 6218-TCR.

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			

- Molecule 5 is a protein called beta chain of the 6218-TCR.

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			

- Molecule 6 is water.

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

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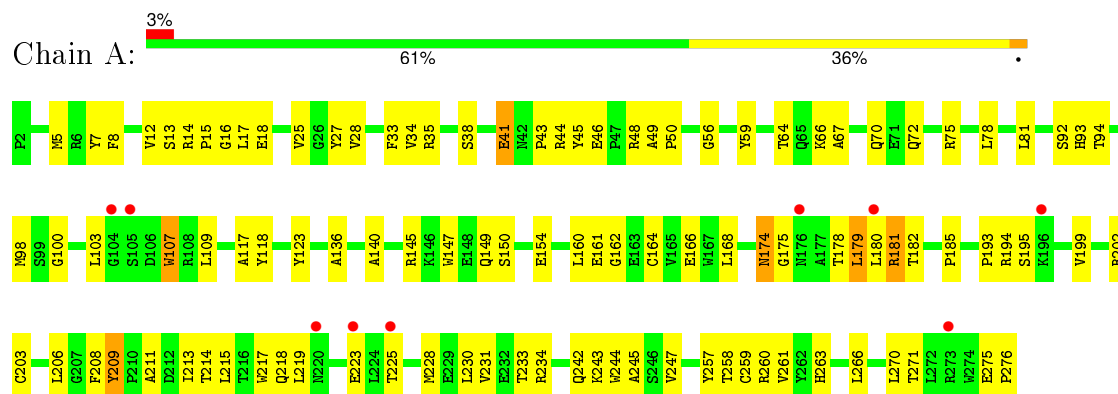
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	1	Total	O	0	0
			1	1		
6	S	1	Total	O	0	0
			1	1		

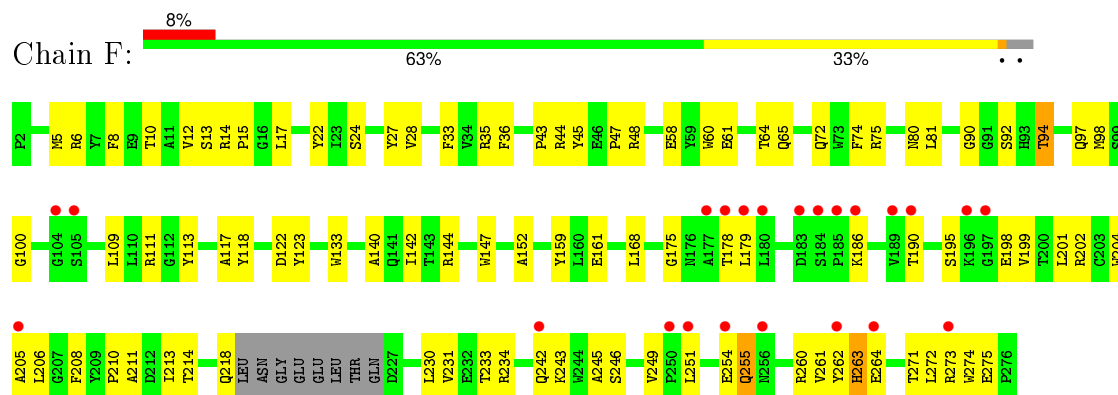
3 Residue-property plots

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

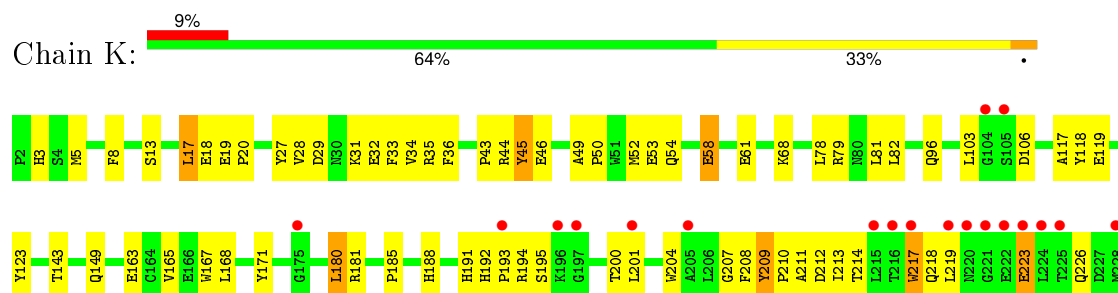
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

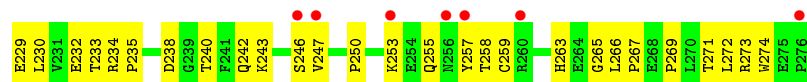


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

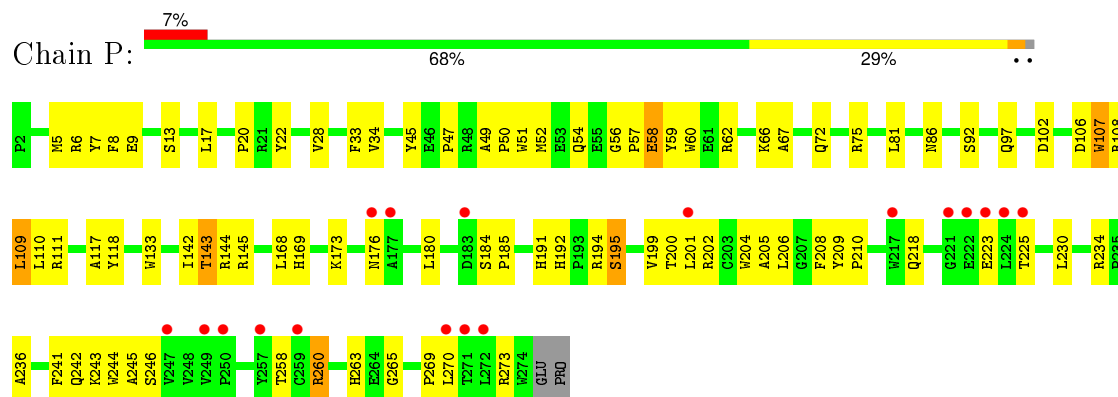


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

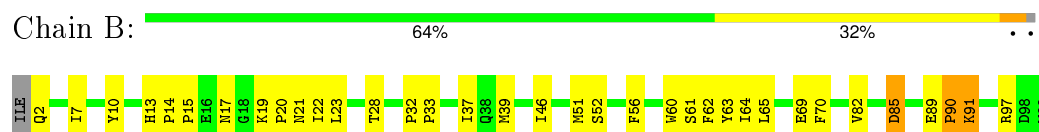




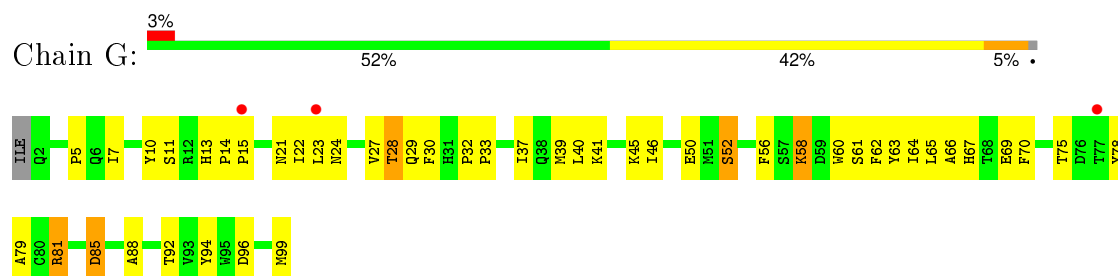
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



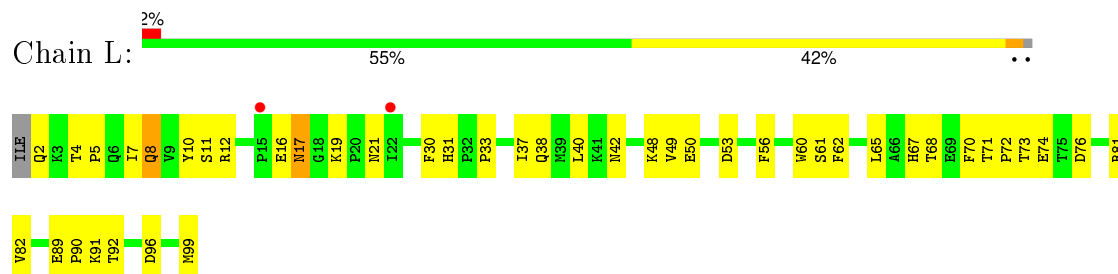
- Molecule 2: Beta-2-microglobulin



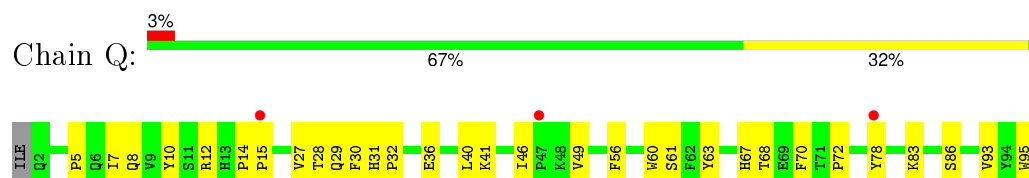
- Molecule 2: Beta-2-microglobulin





- Molecule 2: Beta-2-microglobulin





- Molecule 2: Beta-2-microglobulin



- Chain C: 

- Chain H:  70% 30%
- 

- Chain M:  70% 30%
- 
- | Category | Green (%) | Yellow (%) |
|----------|-----------|------------|
| S1 | 100 | 0 |
| N5 | 0 | 100 |
| F6 | 100 | 0 |
| R7 | 0 | 100 |
| V10 | 0 | 100 |

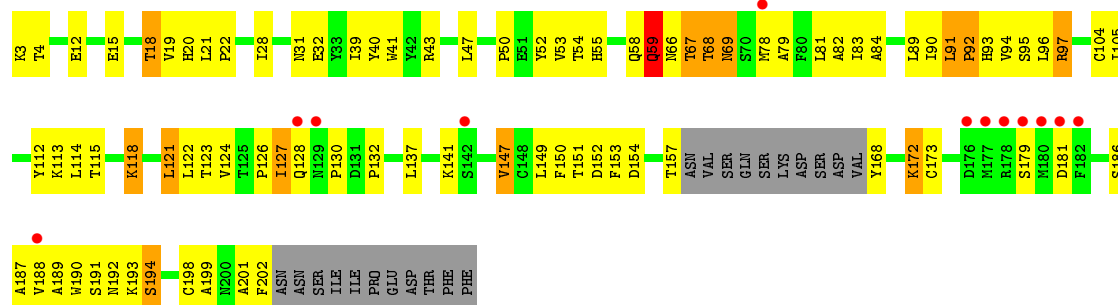
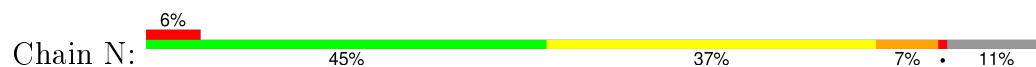
- Chain R:

- Chain D:
-
- 59% 30% 7%

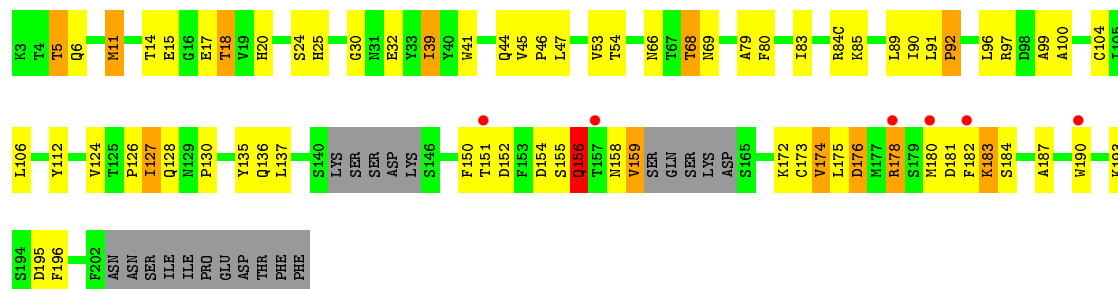
- Chain I:
-
- | Item | Category |
|------|----------|
| K3 | Green |
| T4 | Green |
| M11 | Yellow |
| T14 | Yellow |
| E15 | Yellow |
| G16 | Yellow |
| E17 | Yellow |
| T18 | Yellow |
| V19 | Yellow |
| H20 | Yellow |
| C23 | Green |
| S24 | Yellow |
| H25 | Yellow |
| A26 | Yellow |
| T27 | Yellow |
| I28 | Yellow |
| S29 | Green |
| G30 | Yellow |
| N31 | Yellow |
| E32 | Yellow |
| T33 | Yellow |
| I39 | Orange |
| Y40 | Yellow |
| W41 | Yellow |
| Y42 | Yellow |
| R43 | Yellow |
| Q44 | Yellow |
| V45 | Yellow |
| F46 | Yellow |
| T47 | Red |
| Q48 | Yellow |
| G49 | Yellow |
| P50 | Yellow |
| E51 | Yellow |
| Y52 | Yellow |
| N66 | Yellow |
| T67 | Yellow |
| T68 | Yellow |
| M78 | Yellow |
| A79 | Orange |
| F80 | Yellow |
| L81 | Yellow |
| A82 | Yellow |
| R84C | Yellow |
| L89 | Yellow |
| P92 | Yellow |
| H93 | Orange |
| L96 | Yellow |
| A99 | Yellow |
| I105 | Green |
| L106 | Green |
| S107 | Yellow |
| G108 | Yellow |
| Y112 | Green |
| K113 | Yellow |
| L114 | Yellow |
| T115 | Yellow |
| V124 | Yellow |
| T125 | Yellow |
| P126 | Yellow |
| I127 | Yellow |
| S128 | Yellow |
| Q128 | Red |
| N129 | Yellow |
| P130 | Yellow |
| A133 | Yellow |
| V134 | Yellow |
| L137 | Yellow |
| R138 | Yellow |
| D139 | Yellow |
| D144 | Red |
| V147 | Yellow |
| C148 | Orange |
| L149 | Yellow |
| F150 | Yellow |
| T151 | Yellow |
| D154 | Yellow |
| S155 | Yellow |
| Q156 | Yellow |
| T157 | Yellow |
| N158 | Yellow |
| VAL | Yellow |
| SER | Yellow |
| GLW | Yellow |
| LVS | Yellow |
| ASP | Yellow |
| SER | Yellow |
| D166 | Green |
| D176 | Yellow |
| R177 | Yellow |
| R178 | Yellow |
| S179 | Yellow |
| M180 | Yellow |
| D181 | Yellow |
| F182 | Red |
| K183 | Yellow |
| S184 | Yellow |
| N185 | Yellow |
| S186 | Yellow |



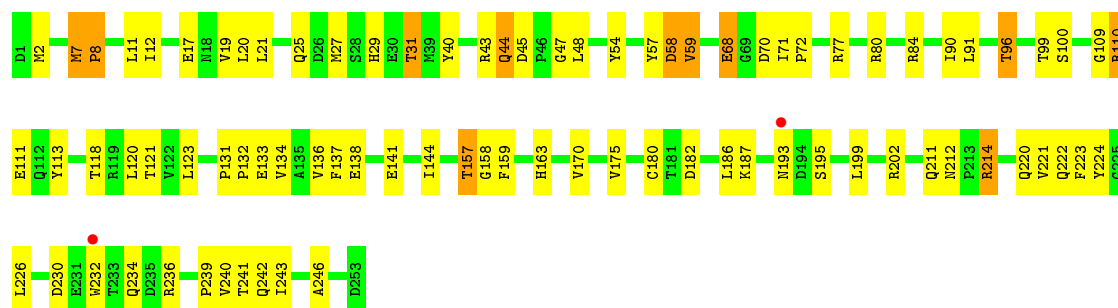
- Molecule 4: alpha chain of the 6218-TCR



- Molecule 4: alpha chain of the 6218-TCR

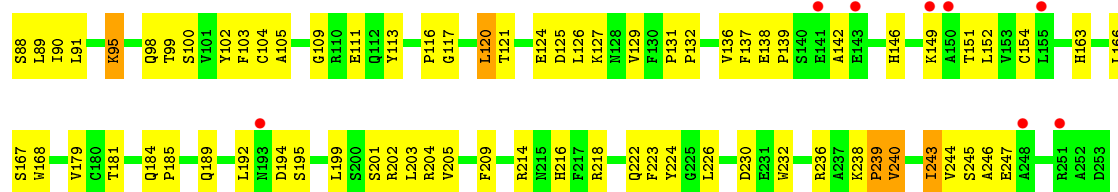


- Molecule 5: beta chain of the 6218-TCR

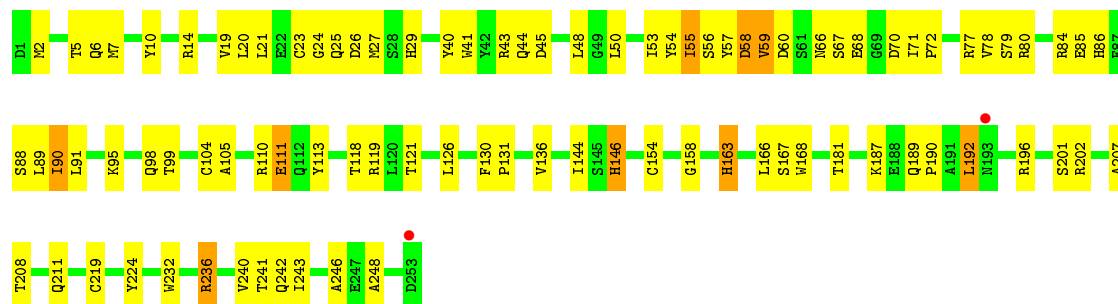


- Molecule 5: beta chain of the 6218-TCR

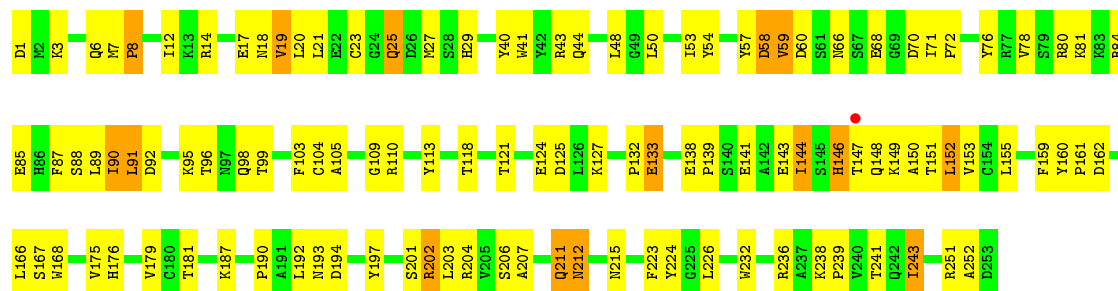




- Molecule 5: beta chain of the 6218-TCR



- Molecule 5: beta chain of the 6218-TCR



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	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.246 , 0.316 0.242 , 0.315	Depositor DCC
R_{free} test set	3545 reflections (5.34%)	DCC
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 , 74.8	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 69960 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.90	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.21	0/2327	0.37	0/3160
1	F	0.20	0/2264	0.36	0/3073
1	K	0.21	0/2327	0.36	0/3160
1	P	0.20	0/2310	0.37	0/3136
2	B	0.21	0/839	0.40	0/1137
2	G	0.21	0/839	0.38	0/1137
2	L	0.21	0/839	0.40	0/1137
2	Q	0.20	0/839	0.39	0/1137
3	C	0.25	0/85	0.40	0/112
3	H	0.23	0/85	0.34	0/112
3	M	0.23	0/85	0.40	0/112
3	R	0.24	0/85	0.36	0/112
4	D	0.22	0/1495	0.41	0/2032
4	I	0.22	0/1497	0.43	0/2036
4	N	0.22	0/1380	0.42	0/1875
4	S	0.22	0/1377	0.41	0/1873
5	E	0.22	0/1992	0.39	0/2702
5	J	0.22	0/1992	0.39	0/2702
5	O	0.22	0/1992	0.38	0/2702
5	T	0.22	0/1992	0.39	0/2702
All	All	0.21	0/26641	0.39	0/36149

There are no bond length outliers.

There are no bond angle outliers.

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	73	0
1	F	2198	0	2072	66	0
1	K	2260	0	2133	74	0
1	P	2244	0	2118	66	0
2	B	813	0	782	26	0
2	G	813	0	782	33	0
2	L	813	0	782	35	0
2	Q	813	0	782	21	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	73	0
4	I	1464	0	1394	98	0
4	N	1350	0	1294	83	0
4	S	1348	0	1286	64	0
5	E	1941	0	1857	63	0
5	J	1941	0	1857	96	0
5	O	1941	0	1857	71	0
5	T	1941	0	1857	102	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
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	956	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 19.

All (956) 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
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
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
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
1:P:6:ARG:HG2	1:P:6:ARG:HH11	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:CG	1:P:6:ARG:HH11	1.94	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:O:144:ILE:HG23	5:O:207:ALA:HB1	1.72	0.70
4:I:133:ALA:HA	4:I:211:THR:HG22	1.73	0.70
4:D:150:PHE:HB3	4:D:153:PHE:CE1	2.26	0.70
4:S:127:ILE:H	4:S:127:ILE:HD12	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:HA	4:N:118:LYS:HE2	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
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
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: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
4:D:144:ASP:HB3	4:D:194:SER:HB3	1.75	0.67
1:P:204:TRP:HE3	1:P:206:LEU:HD11	1.60	0.67
1:A:180:LEU:HD12	1:A:181:ARG:N	2.09	0.67
5:T:151:THR:OG1	5:T:204:ARG:HA	1.94	0.66
4:D:105:ILE:HG21	4:D:114:LEU:HB2	1.77	0.66
5:T:25:GLN:HE22	5:T:29:HIS:N	1.92	0.66
5:J:189:GLN:HB3	5:J:192:LEU:HD13	1.77	0.66
3:C:10:VAL:O	3:C:10:VAL:HG12	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:42:ASN:HD21	2:L:76:ASP:HA	1.60	0.66
1:K:238:ASP:HB3	2:L:12:ARG:HH21	1.60	0.66
4:S:130:PRO:HB3	4:S:154:ASP:HB2	1.76	0.66
3:H:7:ARG:HD2	5:J:109:GLY:O	1.96	0.66
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.30	0.66
2:Q:29:GLN:HA	2:Q:61:SER:HB3	1.77	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
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
5:T:68:GLU:HB3	5:T:72:PRO:HG3	1.79	0.65
1:F:72:GLN:HG2	1:F:75:ARG:HH12	1.60	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
4:N:151:THR:HG22	4:N:186:SER:HB3	1.77	0.64
1:P:192:HIS:HB2	1:P:200:THR:HG23	1.79	0.64
5:J:77:ARG:HB3	5:J:90:ILE:HB	1.78	0.64
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
5:O:136:VAL:HG23	5:O:246:ALA:HB3	1.80	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
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:S:175:LEU:HB2	4:S:184:SER:HB3	1.79	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
5:T:143:GLU:OE1	5:T:150:ALA:HB2	1.98	0.63
5:O:110:ARG:HG2	5:O:111:GLU:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:52:TYR:CB	5:E:111:GLU:HG3	2.30	0.62
2:B:33:PRO:HG3	2:B:62:PHE:CE1	2.34	0.62
4:N:153:PHE:H	4:N:154:ASP:CA	2.12	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
4:I:193:LYS:HG2	4:I:195:ASP:H	1.65	0.61
2:G:13:HIS:HB2	2:G:14:PRO:HD2	1.82	0.61
5:E:214:ARG:HE	5:E:214:ARG:HA	1.65	0.61
5:T:226:LEU:HD13	5:T:239:PRO:HG2	1.82	0.61
1:K:79:ARG:HH12	5:O:59:VAL:HG23	1.65	0.61
1:F:231:VAL:O	1:F:243:LYS:HE3	2.00	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
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
4:I:176:ASP:CG	4:I:177:MET:H	2.03	0.61
1:K:28:VAL:HG23	1:K:33:PHE:CE1	2.36	0.61
5:J:2:MET:HG3	5:J:113:TYR:CE1	2.36	0.61
4:S:80:PHE:HB2	4:S:90:ILE:HB	1.81	0.61
5:J:25:GLN:O	5:J:26:ASP:HB2	1.99	0.61
4:S:183:LYS:HB2	4:S:184:SER:CB	2.24	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
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.36	0.61
5:E:20:LEU:HD23	5:E:90:ILE:HG13	1.83	0.60
1:F:6:ARG:HB2	1:F:27:TYR:HB2	1.82	0.60
5:T:105:ALA:HA	5:T:113:TYR:O	2.00	0.60
2:L:11:SER:HB2	2:L:21:ASN:HD21	1.65	0.60
4:I:30:GLY:HA2	4:I:84(C):ARG:HH12	1.67	0.60
5:J:238:LYS:HE3	5:J:240:VAL:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.84	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
4:N:19:VAL:HG23	4:N:94:VAL:HG11	1.83	0.60
1:K:234:ARG:HD2	2:L:8:GLN:NE2	2.16	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
4:I:178:ARG:H	4:I:179:SER:HB3	1.67	0.59
2:G:27:VAL:HG21	2:G:37:ILE:HD12	1.84	0.59
4:N:153:PHE:N	4:N:154:ASP:HA	2.16	0.59
2:L:96:ASP:HB3	2:L:99:MET:HB2	1.84	0.59
4:I:130:PRO:HG3	4:I:154:ASP:HB2	1.84	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
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:D:68:THR:HG21	4:I:68:THR:HB	1.85	0.59
1:F:80:ASN:HA	1:P:86:ASN:HD21	1.68	0.59
4:I:78:MET:O	4:I:79:ALA:HB3	2.02	0.59
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.37	0.59
5:J:48:LEU:H	5:J:48:LEU:HD12	1.68	0.59
1:A:149:GLN:O	5:E:110:ARG:HD2	2.03	0.59
4:I:178:ARG:HB3	4:I:180:MET:HB2	1.84	0.59
1:P:176:ASN:HA	1:P:180:LEU:HD13	1.85	0.59
5:E:187:LYS:HB3	5:E:195:SER:OG	2.03	0.59
1:P:81:LEU:HB3	1:P:118:TYR:CE2	2.38	0.59
5:J:21:LEU:HD12	5:J:89:LEU:HD23	1.85	0.59
5:J:11:LEU:HD23	5:J:120:LEU:HD12	1.84	0.58
1:A:275:GLU:HB3	1:A:276:PRO:HD2	1.85	0.58
5:E:2:MET:HE1	5:E:29:HIS:HE1	1.68	0.58
4:N:79:ALA:HB2	4:N:91:LEU:HD13	1.84	0.58
4:D:52:TYR:HB2	5:E:111:GLU:HG3	1.85	0.58
5:J:6:GLN:HE21	5:J:104:CYS:H	1.48	0.58
1:F:15:PRO:HA	1:F:90:GLY:O	2.04	0.58
1:K:50:PRO:O	1:K:53:GLU:HG2	2.03	0.58
2:B:13:HIS:HB2	2:B:21:ASN:ND2	2.19	0.58
5:T:139:PRO:HD3	5:T:152:LEU:HD12	1.86	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
4:S:25:HIS:NE2	4:S:39:ILE:HD12	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:206:ILE:HG13	4:D:207:ILE:N	2.11	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
5:E:70:ASP:C	5:E:72:PRO:HD3	2.24	0.58
2:L:19:LYS:H	2:L:72:PRO:HD2	1.69	0.58
1:K:5:MET:HB2	1:K:168:LEU:HD13	1.85	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
1:F:195:SER:OG	1:F:198:GLU:HB2	2.04	0.58
4:N:66:ASN:CG	4:N:67:THR:H	2.05	0.58
1:K:263:HIS:CD2	1:K:265:GLY:H	2.22	0.58
4:D:128:GLN:HG2	4:D:183:LYS:HG3	1.84	0.58
4:N:95:SER:HB3	4:N:97:ARG:HD3	1.85	0.57
4:I:130:PRO:CG	4:I:154:ASP:HB2	2.33	0.57
4:D:21:LEU:HD12	4:D:89:LEU:HD23	1.85	0.57
2:G:39:MET:HB3	2:G:46:ILE:HD12	1.86	0.57
5:T:168:TRP:HD1	5:T:179:VAL:HG13	1.68	0.57
4:I:158:ASN:H	4:I:158:ASN:HD22	1.52	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
4:S:25:HIS:HE1	4:S:104:CYS:SG	2.27	0.57
2:G:7:ILE:HG22	2:G:27:VAL:HG22	1.87	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: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:150:PHE:HB3	4:D:153:PHE:HE1	1.67	0.56
1:P:202:ARG:HB3	1:P:246:SER:HB3	1.87	0.56
1:P:8:PHE:HB3	2:Q:56:PHE:CE2	2.39	0.56
4:D:26:ALA:HA	4:D:85:LYS:HA	1.87	0.56
5:T:57:TYR:O	5:T:58:ASP:HB2	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:2:MET:HE1	5:O:29:HIS:HE1	1.71	0.56
5:E:43:ARG:NH2	5:E:100:SER:HB2	2.18	0.56
5:O:70:ASP:O	5:O:71:ILE:HD13	2.05	0.56
4:I:209:GLU:CA	4:I:210:ASP:HB3	2.35	0.56
5:E:21:LEU:HD22	5:E:118:THR:HG21	1.87	0.56
1:K:167:TRP:HB3	1:K:171:TYR:CE2	2.40	0.56
5:E:131:PRO:HD3	5:E:239:PRO:HB3	1.88	0.56
2:B:52:SER:HB3	2:B:65:LEU:H	1.71	0.56
5:J:43:ARG:HH21	5:J:100:SER:HB2	1.71	0.56
5:J:70:ASP:C	5:J:72:PRO:HD3	2.26	0.56
5:J:6:GLN:HE22	5:J:103:PHE:HA	1.70	0.56
1:A:16:GLY:O	1:A:18:GLU:HG3	2.06	0.56
1:A:8:PHE:HB3	2:B:56:PHE:CZ	2.41	0.56
5:J:95:LYS:HB2	5:J:98:GLN:HG3	1.88	0.56
4:I:210:ASP:CB	4:I:211:THR:HG23	2.36	0.55
2:G:11:SER:HB2	2:G:21:ASN:ND2	2.21	0.55
5:J:56:SER:HB2	5:J:87:PHE:CZ	2.41	0.55
4:N:54:THR:HG23	4:N:81:LEU:HD23	1.88	0.55
2:L:11:SER:HB2	2:L:21:ASN:ND2	2.20	0.55
1:F:14:ARG:HB3	1:F:17:LEU:HD13	1.88	0.55
5:T:243:ILE:HD13	5:T:243:ILE:N	2.22	0.55
1:A:260:ARG:HG2	1:A:271:THR:HG22	1.88	0.55
4:N:149:LEU:HD11	4:N:186:SER:HB2	1.89	0.55
4:I:50:PRO:HG2	5:J:50:LEU:HD22	1.88	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
5:O:2:MET:CE	5:O:29:HIS:HE1	2.20	0.55
1:K:103:LEU:HD11	1:K:165:VAL:HG13	1.89	0.55
4:N:66:ASN:O	4:N:67:THR:HB	2.08	0.54
3:C:3:LEU:HD12	3:C:4:GLU:H	1.72	0.54
1:F:251:LEU:HD12	1:F:254:GLU:OE1	2.08	0.54
5:E:54:TYR:HA	5:E:68:GLU:O	2.07	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:D:29:SER:C	4:D:31:ASN:H	2.10	0.54
4:I:183:LYS:O	4:I:184:SER:HB3	2.08	0.54
4:I:127:ILE:HD12	4:I:127:ILE:H	1.73	0.54
4:N:19:VAL:HG23	4:N:94:VAL:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:P:13:SER:HA	1:P:20:PRO:HB3	1.90	0.54
2:L:49:VAL:HG22	2:L:68:THR:HB	1.89	0.54
1:K:219:LEU:HD13	1:K:257:TYR:CE2	2.42	0.54
5:J:40:TYR:HB2	5:J:105:ALA:HB3	1.90	0.54
4:S:96:LEU:HA	4:S:124:VAL:HG11	1.90	0.54
1:P:72:GLN:HG3	1:P:75:ARG:NH2	2.23	0.54
4:N:168:TYR:CD2	4:N:191:SER:HB3	2.43	0.54
1:K:211:ALA:HB1	1:K:233:THR:HG21	1.89	0.54
1:K:263:HIS:CD2	1:K:266:LEU:HD13	2.43	0.54
2:B:33:PRO:HG3	2:B:62:PHE:CZ	2.43	0.54
4:N:3:LYS:NZ	4:N:3:LYS:HB2	2.23	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
5:J:222:GLN:OE1	5:J:243:ILE:HG23	2.08	0.54
5:J:154:CYS:HB2	5:J:168:TRP:CH2	2.43	0.54
1:K:68:LYS:HA	1:K:68:LYS:HE2	1.90	0.54
5:T:168:TRP:CD1	5:T:179:VAL:HG13	2.43	0.53
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
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:F:213:ILE:HD11	1:F:261:VAL:HG13	1.89	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
4:I:46:PRO:O	4:I:47:LEU:HG	2.08	0.53
1:K:185:PRO:HD2	1:K:266:LEU:HD11	1.88	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
1:F:14:ARG:HD2	1:F:17:LEU:HD22	1.90	0.53
1:K:96:GLN:OE1	2:L:31:HIS:HE1	1.92	0.53
5:T:143:GLU:CD	5:T:150:ALA:HB2	2.29	0.53
4:I:149:LEU:HG	4:I:151:THR:HG23	1.91	0.53
4:S:18:THR:HA	4:S:92:PRO:O	2.08	0.53
5:O:95:LYS:HB2	5:O:98:GLN:HG3	1.91	0.53
5:O:207:ALA:O	5:O:211:GLN:HG2	2.09	0.53
4:I:151:THR:HG22	4:I:186:SER:CB	2.38	0.53
1:F:234:ARG:HD2	2:G:10:TYR:CE1	2.43	0.53
2:L:30:PHE:CE1	2:L:62:PHE:HB2	2.44	0.53
4:I:178:ARG:NH2	5:J:204:ARG:HD3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:193:LYS:HD2	4:N:194:SER:N	2.24	0.53
4:D:46:PRO:O	4:D:47:LEU:HB2	2.09	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
5:E:77:ARG:HG3	5:E:90:ILE:HB	1.89	0.52
2:B:89:GLU:HB2	2:B:90:PRO:HD2	1.90	0.52
1:P:133:TRP:HB2	1:P:144:ARG:HG3	1.90	0.52
5:T:7:MET:HB3	5:T:8:PRO:CD	2.31	0.52
4:I:184:SER:HB2	5:J:204:ARG:HH21	1.73	0.52
4:I:134:VAL:HG12	4:I:211:THR:HG21	1.90	0.52
4:S:14:THR:H	4:S:17:GLU:CD	2.13	0.52
1:P:8:PHE:HB3	2:Q:56:PHE:CZ	2.44	0.52
1:F:12:VAL:HG13	1:F:94:THR:HG23	1.92	0.52
5:E:170:VAL:HG23	5:E:175:VAL:HG21	1.91	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:121:LEU:HD21	4:N:123:THR:HG23	1.91	0.52
1:P:51:TRP:O	1:P:54:GLN:HG2	2.09	0.52
4:N:172:LYS:HA	4:N:187:ALA:HB2	1.91	0.52
5:T:68:GLU:HB3	5:T:72:PRO:CG	2.39	0.52
4:N:90:ILE:O	4:N:91:LEU:HB2	2.09	0.52
4:N:105:ILE:HD13	4:N:114:LEU:HD13	1.92	0.52
5:O:126:LEU:HD12	5:O:126:LEU:H	1.74	0.52
5:T:232:TRP:HB2	5:T:238:LYS:HE2	1.92	0.52
1:A:162:GLY:O	1:A:166:GLU:HG2	2.09	0.52
5:T:25:GLN:HE22	5:T:29:HIS:H	1.55	0.52
4:D:170:THR:HG23	4:D:188:VAL:H	1.75	0.52
5:O:24:GLY:HA2	5:O:85:GLU:O	2.09	0.52
4:N:54:THR:HB	4:N:69:ASN:OD1	2.09	0.52
4:S:45:VAL:HG22	4:S:100:ALA:HB2	1.90	0.52
4:S:46:PRO:O	4:S:47:LEU:HB2	2.10	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
5:O:208:THR:HA	5:O:211:GLN:HG2	1.91	0.52
5:J:238:LYS:HE3	5:J:240:VAL:CG2	2.40	0.52
4:D:128:GLN:HG2	4:D:183:LYS:CG	2.40	0.51
5:T:6:GLN:HE22	5:T:103:PHE:HA	1.75	0.51
4:N:67:THR:OG1	4:S:68:THR:HG21	2.10	0.51
5:T:19:VAL:HG13	5:T:91:LEU:CD1	2.39	0.51
4:I:209:GLU:HA	4:I:210:ASP:O	2.09	0.51
5:T:147:THR:O	5:T:149:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:95:TRP:CD1	2:Q:96:ASP:N	2.77	0.51
4:D:201:ALA:O	4:D:202:PHE:HB3	2.11	0.51
1:A:81:LEU:HB3	1:A:118:TYR:CE2	2.46	0.51
4:I:207:ILE:O	4:I:207:ILE:HG23	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
5:E:186:LEU:H	5:E:186:LEU:HD23	1.75	0.51
5:O:66:ASN:HD22	5:O:78:VAL:CG2	2.18	0.51
2:G:33:PRO:HG3	2:G:62:PHE:CZ	2.45	0.51
2:G:24:ASN:ND2	2:G:65:LEU:HD11	2.25	0.51
2:L:33:PRO:HG3	2:L:62:PHE:CE1	2.46	0.51
1:A:208:PHE:CE2	1:A:242:GLN:HA	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
1:K:58:GLU:H	1:K:58:GLU:CD	2.14	0.51
4:S:175:LEU:O	4:S:176:ASP:HB2	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
5:J:184:GLN:OE1	5:J:185:PRO:HD2	2.11	0.51
2:L:40:LEU:HD21	2:L:81:ARG:NH2	2.26	0.51
1:F:263:HIS:CG	1:F:264:GLU:N	2.79	0.51
1:K:31:LYS:HD2	1:K:209:TYR:OH	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:P:263:HIS:CD2	1:P:265:GLY:H	2.28	0.51
5:O:71:ILE:N	5:O:72:PRO:HD3	2.26	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:E:99:THR:OG1	5:E:121:THR:HA	2.11	0.50
4:N:113:LYS:HE3	5:O:57:TYR:OH	2.11	0.50
4:D:68:THR:HG21	4:I:68:THR:CB	2.41	0.50
5:J:71:ILE:N	5:J:72:PRO:HD3	2.26	0.50
4:D:112:TYR:CE1	5:E:31:THR:HG21	2.47	0.50
3:C:7:ARG:HD2	5:E:109:GLY:O	2.11	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
5:T:153:VAL:HG22	5:T:202:ARG:HB3	1.94	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
1:A:182:THR:HB	1:A:209:TYR:O	2.11	0.50
4:S:11:MET:HE2	4:S:11:MET:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:27:VAL:HG12	2:Q:30:PHE:CD2	2.47	0.50
2:G:33:PRO:HG3	2:G:62:PHE:CE1	2.46	0.50
2:B:51:MET:HB3	2:B:64:ILE:HD11	1.93	0.50
5:O:55:ILE:HD13	5:O:56:SER:N	2.26	0.50
1:K:163:GLU:O	1:K:167:TRP:HD1	1.94	0.50
1:K:117:ALA:HB2	2:L:60:TRP:CE2	2.47	0.50
4:D:141:LYS:HA	4:D:141:LYS:HE3	1.94	0.50
1:P:56:GLY:O	1:P:59:TYR:HB3	2.12	0.50
1:K:81:LEU:HD13	1:K:118:TYR:CD1	2.47	0.50
5:J:80:ARG:HD2	5:J:86:HIS:O	2.11	0.50
1:F:206:LEU:HD12	1:F:206:LEU:N	2.26	0.50
4:I:206:ILE:HG23	4:I:208:PRO:HD3	1.94	0.50
4:S:183:LYS:CA	4:S:184:SER:HB2	2.43	0.49
5:J:226:LEU:O	5:J:240:VAL:HA	2.11	0.49
5:T:58:ASP:O	5:T:59:VAL:C	2.50	0.49
5:O:5:THR:O	5:O:23:CYS:HA	2.11	0.49
2:B:7:ILE:HD12	2:B:91:LYS:HG2	1.93	0.49
1:K:232:GLU:HA	1:K:243:LYS:HZ2	1.76	0.49
5:O:126:LEU:O	5:O:232:TRP:HZ3	1.95	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CZ2	2.47	0.49
1:K:103:LEU:HD12	1:K:168:LEU:HD23	1.93	0.49
2:B:15:PRO:HG2	2:B:97:ARG:HB2	1.94	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:NH1	1:K:181:ARG:HB3	2.27	0.49
4:N:186:SER:OG	5:O:202:ARG:HD2	2.13	0.49
1:F:133:TRP:HB2	1:F:144:ARG:HG3	1.94	0.49
4:N:153:PHE:H	4:N:154:ASP:HB2	1.77	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
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
5:E:2:MET:CE	5:E:29:HIS:HE1	2.25	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
2:B:28:THR:HG22	2:B:63:TYR:HB2	1.95	0.49
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:N	5:T:95:LYS:HD2	2.28	0.49
4:D:114:LEU:HD12	4:D:114:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:232:GLU:HA	1:K:243:LYS:NZ	2.28	0.48
5:T:151:THR:HG22	5:T:152:LEU:HD22	1.95	0.48
5:T:59:VAL:O	5:T:80:ARG:HB3	2.13	0.48
5:T:58:ASP:OD1	5:T:84:ARG:HD3	2.12	0.48
4:N:20:HIS:CE1	4:S:18:THR:HG21	2.48	0.48
1:K:52:MET:C	1:K:54:GLN:H	2.17	0.48
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
4:N:149:LEU:HG	4:N:151:THR:HG23	1.94	0.48
1:K:81:LEU:HD21	3:M:10:VAL:HG11	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
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
2:G:32:PRO:HD2	2:G:85:ASP:OD1	2.14	0.48
5:T:166:LEU:HD23	5:T:167:SER:N	2.27	0.48
4:D:134:VAL:HA	4:D:149:LEU:O	2.13	0.48
2:B:37:ILE:HG12	2:B:82:VAL:HG22	1.94	0.48
4:N:58:GLN:O	4:N:59:GLN:C	2.51	0.48
5:E:243:ILE:HG13	5:E:243:ILE:O	2.13	0.48
4:I:66:ASN:HD22	4:I:82:ALA:HA	1.78	0.48
1:P:117:ALA:HB2	2:Q:60:TRP:CE2	2.49	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:S:41:TRP:CE3	4:S:89:LEU:HD22	2.48	0.48
4:N:41:TRP:CE3	4:N:89:LEU:HD22	2.48	0.48
2:G:96:ASP:OD1	2:G:99:MET:HB2	2.14	0.48
1:F:117:ALA:HB2	2:G:60:TRP:CZ2	2.48	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
1:F:111:ARG:HD3	1:F:113:TYR:OH	2.14	0.48
5:T:144:ILE:H	5:T:144:ILE:HD12	1.78	0.48
5:T:99:THR:O	5:T:99:THR:HG22	2.14	0.48
4:N:112:TYR:HB3	5:O:40:TYR:OH	2.13	0.48
4:S:112:TYR:HB3	5:T:40:TYR:OH	2.14	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
2:G:40:LEU:HD11	2:G:81:ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:6:GLN:HE22	5:J:104:CYS:H	1.58	0.48
4:I:210:ASP:HA	4:I:211:THR:HA	1.58	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
4:D:202:PHE:CE2	4:D:207:ILE:HD11	2.49	0.47
1:A:103:LEU:HD13	1:A:168:LEU:HD23	1.96	0.47
5:O:25:GLN:NE2	5:O:29:HIS:N	2.61	0.47
4:N:191:SER:HB2	4:N:192:ASN:CG	2.34	0.47
4:I:105:ILE:HG21	4:I:114:LEU:HB2	1.95	0.47
4:D:168:TYR:O	4:D:189:ALA:HA	2.14	0.47
4:N:118:LYS:O	4:N:118:LYS:HD3	2.14	0.47
5:T:70:ASP:O	5:T:71:ILE:HD13	2.15	0.47
1:K:200:THR:O	1:K:201:LEU:HD13	2.14	0.47
2:Q:70:PHE:CE2	2:Q:72:PRO:HG3	2.49	0.47
1:F:218:GLN:NE2	1:F:260:ARG:HH11	2.03	0.47
1:A:150:SER:HA	5:E:110:ARG:HG2	1.97	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
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
4:I:112:TYR:HB3	5:J:40:TYR:OH	2.14	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
5:J:59:VAL:CG1	5:J:60:ASP:H	2.13	0.47
5:O:6:GLN:HE22	5:O:104:CYS:H	1.57	0.47
2:G:10:TYR:O	2:G:23:LEU:HD12	2.14	0.47
4:I:206:ILE:O	4:I:207:ILE:C	2.52	0.47
4:S:137:LEU:HD12	5:T:138:GLU:O	2.14	0.47
1:K:36:PHE:HB2	1:K:45:TYR:CE1	2.49	0.47
4:S:53:VAL:HG23	4:S:54:THR:N	2.28	0.47
5:T:18:ASN:OD1	5:T:92:ASP:HA	2.14	0.47
1:P:191:HIS:NE2	1:P:199:VAL:HG11	2.29	0.47
4:D:206:ILE:CG1	4:D:207:ILE:N	2.76	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
4:I:46:PRO:HB2	4:I:47:LEU:HD23	1.97	0.47
1:P:202:ARG:HA	1:P:245:ALA:O	2.15	0.47
4:I:78:MET:O	4:I:79:ALA:CB	2.62	0.47
5:O:154:CYS:HB2	5:O:168:TRP:CH2	2.49	0.47
2:B:28:THR:HG22	2:B:63:TYR:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:4:VAL:O	5:J:116:PRO:HD3	2.13	0.47
4:I:209:GLU:CA	4:I:210:ASP:CB	2.92	0.47
1:F:123:TYR:CZ	1:F:140:ALA:HA	2.49	0.47
4:N:3:LYS:HG3	4:N:4:THR:H	1.79	0.47
4:S:137:LEU:HD22	4:S:137:LEU:N	2.30	0.47
4:I:197:ALA:O	4:I:201:ALA:HB3	2.14	0.47
4:S:150:PHE:HB2	4:S:187:ALA:HB3	1.97	0.47
5:E:12:ILE:HD11	5:E:123:LEU:HD12	1.97	0.47
4:S:20:HIS:CD2	4:S:90:ILE:HG13	2.50	0.47
5:J:129:VAL:HG11	5:J:226:LEU:CD2	2.45	0.47
4:S:32:GLU:HG2	4:S:106:LEU:HB3	1.97	0.47
4:D:158:ASN:C	4:D:160:SER:H	2.18	0.46
5:O:23:CYS:O	5:O:86:HIS:HA	2.15	0.46
4:N:105:ILE:HG21	4:N:114:LEU:HD13	1.96	0.46
1:A:72:GLN:HG3	1:A:75:ARG:NH2	2.30	0.46
5:T:146:HIS:C	5:T:148:GLN:H	2.18	0.46
5:T:14:ARG:O	5:T:17:GLU:HB2	2.15	0.46
5:J:223:PHE:CD1	5:J:224:TYR:N	2.83	0.46
1:A:35:ARG:HB3	1:A:48:ARG:HD3	1.97	0.46
2:G:79:ALA:HB2	2:G:94:TYR:CD2	2.50	0.46
4:S:39:ILE:HD11	4:S:41:TRP:HE1	1.79	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:D:137:LEU:HB3	5:E:138:GLU:O	2.15	0.46
4:N:95:SER:CB	4:N:97:ARG:HD3	2.46	0.46
4:N:67:THR:OG1	4:N:68:THR:N	2.48	0.46
4:I:178:ARG:HH21	5:J:204:ARG:HD3	1.79	0.46
4:I:4:THR:HG22	4:I:25:HIS:HB3	1.97	0.46
5:T:159:PHE:CE2	5:T:162:ASP:HA	2.50	0.46
2:B:14:PRO:HA	2:B:15:PRO:HD3	1.81	0.46
1:K:35:ARG:CZ	2:L:53:ASP:HB3	2.46	0.46
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
4:I:28:ILE:HG13	4:I:32:GLU:HG3	1.96	0.46
5:J:139:PRO:HD3	5:J:152:LEU:HG	1.96	0.46
2:Q:31:HIS:CD2	2:Q:32:PRO:HA	2.51	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
1:P:258:THR:HG22	1:P:273:ARG:HG2	1.97	0.46
4:N:188:VAL:HG12	4:N:189:ALA:N	2.30	0.46
4:N:173:CYS:HB3	5:O:202:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:124:VAL:HG13	4:S:124:VAL:O	2.14	0.46
4:D:149:LEU:HG	4:D:151:THR:HG23	1.97	0.46
4:S:156:GLN:HE22	4:S:158:ASN:CG	2.18	0.46
4:D:208:PRO:C	4:D:210:ASP:H	2.19	0.46
4:I:139:ASP:HA	5:J:137:PHE:HA	1.98	0.46
1:P:143:THR:HG21	3:R:10:VAL:HG13	1.97	0.46
5:O:2:MET:CE	5:O:29:HIS:CE1	2.98	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
4:I:128:GLN:NE2	4:I:182:PHE:HD1	2.13	0.46
5:O:243:ILE:O	5:O:243:ILE:HD12	2.15	0.46
4:N:50:PRO:HG3	5:O:50:LEU:CD1	2.40	0.46
5:T:76:TYR:CE1	5:T:91:LEU:HD23	2.50	0.46
1:P:202:ARG:O	1:P:204:TRP:HD1	1.99	0.46
5:J:25:GLN:NE2	5:J:29:HIS:N	2.62	0.46
1:A:234:ARG:HD2	1:A:242:GLN:OE1	2.16	0.46
1:P:234:ARG:HD3	2:Q:8:GLN:NE2	2.30	0.46
5:O:130:PHE:CB	5:O:196:ARG:HH11	2.29	0.46
5:O:41:TRP:CE2	5:O:89:LEU:HB2	2.51	0.46
4:I:209:GLU:HA	4:I:210:ASP:CB	2.45	0.46
4:D:41:TRP:CG	4:D:89:LEU:HD13	2.50	0.46
1:K:17:LEU:O	1:K:19:GLU:N	2.49	0.46
1:F:202:ARG:HA	1:F:245:ALA:O	2.16	0.46
1:P:205:ALA:C	1:P:206:LEU:HD12	2.36	0.46
1:A:5:MET:CE	1:A:7:TYR:HE2	2.29	0.46
1:K:234:ARG:HB3	2:L:10:TYR:CZ	2.51	0.46
5:E:96:THR:O	5:E:99:THR:HG22	2.16	0.46
4:I:114:LEU:O	4:I:114:LEU:HD12	2.16	0.46
1:F:175:GLY:O	1:F:178:THR:HG22	2.16	0.46
3:R:3:LEU:HD12	3:R:4:GLU:H	1.80	0.46
5:E:223:PHE:O	5:E:241:THR:HG23	2.16	0.46
1:F:190:THR:CG2	1:F:202:ARG:HB2	2.46	0.45
1:P:81:LEU:HD13	1:P:118:TYR:CD2	2.51	0.45
5:E:99:THR:O	5:E:99:THR:HG23	2.16	0.45
2:L:4:THR:HG23	2:L:5:PRO:HD2	1.97	0.45
4:I:4:THR:CG2	4:I:106:LEU:HG	2.46	0.45
4:D:159:VAL:O	4:D:160:SER:C	2.54	0.45
5:O:10:TYR:HE1	5:O:119:ARG:HE	1.63	0.45
5:O:25:GLN:O	5:O:26:ASP:HB2	2.17	0.45
1:F:213:ILE:HG12	1:F:214:THR:N	2.32	0.45
4:N:193:LYS:HE2	4:N:193:LYS:HB3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:180:MET:O	4:S:181:ASP:HB2	2.17	0.45
5:E:133:GLU:O	5:E:157:THR:HG23	2.17	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
4:I:27:THR:HG22	4:I:27:THR:O	2.16	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:F:211:ALA:HB1	1:F:233:THR:HG21	1.99	0.45
1:A:70:GLN:HE22	3:C:5:ASN:HB2	1.81	0.45
4:D:128:GLN:HG2	4:D:183:LYS:CD	2.47	0.45
2:G:21:ASN:CG	2:G:22:ILE:H	2.20	0.45
4:S:91:LEU:HA	4:S:92:PRO:HD2	1.70	0.45
1:F:271:THR:C	1:F:272:LEU:HD12	2.37	0.45
1:A:49:ALA:HB1	1:A:50:PRO:HD2	1.98	0.45
4:S:178:ARG:C	4:S:178:ARG:HD3	2.36	0.45
5:O:126:LEU:N	5:O:126:LEU:HD12	2.32	0.45
4:S:6:GLN:OE1	4:S:104:CYS:HB3	2.17	0.45
5:J:48:LEU:N	5:J:48:LEU:HD12	2.31	0.45
5:T:59:VAL:HG13	5:T:81:LYS:O	2.17	0.45
2:G:11:SER:HB2	2:G:21:ASN:HD22	1.82	0.45
1:F:61:GLU:HA	1:F:64:THR:HG22	1.97	0.45
1:P:33:PHE:HD2	1:P:52:MET:HG3	1.81	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:70:ASP:C	5:O:72:PRO:HD3	2.37	0.45
5:E:2:MET:HE2	5:E:2:MET:HB3	1.70	0.45
5:T:27:MET:HG3	5:T:29:HIS:CD2	2.52	0.45
1:K:49:ALA:HB1	1:K:50:PRO:HD2	1.98	0.45
1:P:45:TYR:HE2	1:P:67:ALA:HB2	1.79	0.45
1:K:223:GLU:HG2	1:K:223:GLU:H	1.45	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
1:K:44:ARG:O	1:K:46:GLU:HG3	2.17	0.45
4:I:156:GLN:O	4:I:157:THR:HG22	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:K:234:ARG:HB3	2:L:10:TYR:OH	2.17	0.45
1:K:209:TYR:C	1:K:209:TYR:CD2	2.91	0.45
1:F:274:TRP:CG	1:F:275:GLU:N	2.85	0.45
1:A:109:LEU:CD1	1:A:161:GLU:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:156:GLN:HE22	4:S:158:ASN:ND2	2.16	0.44
1:P:33:PHE:CD2	1:P:34:VAL:HG13	2.52	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
1:P:218:GLN:HE22	1:P:260:ARG:HH11	1.65	0.44
1:K:192:HIS:HA	1:K:193:PRO:HD3	1.78	0.44
1:F:12:VAL:HG22	1:F:94:THR:HG22	2.00	0.44
4:D:80:PHE:HB3	4:I:80:PHE:CD1	2.52	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
4:N:137:LEU:HD12	4:N:137:LEU:N	2.32	0.44
5:J:59:VAL:O	5:J:80:ARG:HB3	2.17	0.44
1:F:190:THR:HG22	1:F:202:ARG:HB2	1.99	0.44
5:E:25:GLN:NE2	5:E:29:HIS:N	2.65	0.44
5:O:136:VAL:HG23	5:O:246:ALA:CB	2.45	0.44
2:L:81:ARG:HD3	2:L:92:THR:OG1	2.17	0.44
5:E:57:TYR:O	5:E:58:ASP:HB2	2.18	0.44
5:O:2:MET:HE2	5:O:2:MET:HB3	1.49	0.44
5:O:43:ARG:HB3	5:O:53:ILE:HD11	1.98	0.44
4:I:129:ASN:HA	4:I:130:PRO:HD3	1.72	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
5:T:43:ARG:HB3	5:T:53:ILE:HD11	1.98	0.44
2:L:37:ILE:HG12	2:L:82:VAL:HG12	1.99	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:175:VAL:HG22	5:T:176:HIS:N	2.32	0.44
5:T:181:THR:HG23	5:T:201:SER:HB2	1.99	0.44
1:A:56:GLY:O	1:A:59:TYR:HB3	2.18	0.44
4:N:201:ALA:O	4:N:202:PHE:HB3	2.18	0.44
1:F:199:VAL:O	1:F:249:VAL:HG22	2.18	0.44
4:N:153:PHE:N	4:N:154:ASP:CA	2.77	0.44
1:A:234:ARG:HD3	2:B:10:TYR:CE1	2.52	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:D:168:TYR:HD2	4:D:190:TRP:CE2	2.35	0.44
1:A:185:PRO:HD3	1:A:263:HIS:CD2	2.53	0.44
5:E:44:GLN:HG3	5:E:44:GLN:O	2.17	0.44
4:N:153:PHE:HB3	4:N:157:THR:O	2.18	0.44
1:K:8:PHE:HB3	2:L:56:PHE:CE2	2.52	0.44
4:I:179:SER:CA	4:I:180:MET:HB2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:21:LEU:HD22	5:T:118:THR:HG21	2.00	0.44
4:I:147:VAL:HG21	4:I:188:VAL:HG13	1.99	0.44
1:P:194:ARG:HG3	1:P:195:SER:N	2.32	0.44
4:N:92:PRO:HB3	4:S:66:ASN:HD21	1.82	0.44
5:J:218:ARG:HG2	5:J:245:SER:OG	2.17	0.44
4:S:173:CYS:HB2	5:T:202:ARG:NH1	2.24	0.44
4:N:52:TYR:CD2	5:O:111:GLU:HB3	2.53	0.44
5:T:41:TRP:HD1	5:T:87:PHE:CE2	2.36	0.44
4:D:141:LYS:O	4:D:142:SER:C	2.57	0.44
4:D:167:VAL:HG11	4:D:200:ASN:HB3	2.00	0.44
1:A:94:THR:O	1:A:118:TYR:HD1	2.01	0.43
1:K:201:LEU:HD22	1:K:201:LEU:N	2.33	0.43
1:K:36:PHE:HB2	1:K:45:TYR:CD1	2.53	0.43
5:T:223:PHE:O	5:T:241:THR:HA	2.18	0.43
4:I:41:TRP:CE3	4:I:89:LEU:HD13	2.53	0.43
1:F:159:TYR:CG	3:H:3:LEU:HD13	2.53	0.43
4:S:84(C):ARG:O	4:S:85:LYS:HB2	2.18	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:90:ILE:HD12	4:S:90:ILE:N	2.33	0.43
1:A:15:PRO:HD3	1:A:92:SER:OG	2.19	0.43
4:S:182:PHE:O	4:S:183:LYS:HB3	2.18	0.43
1:K:263:HIS:HD2	1:K:266:LEU:HD13	1.81	0.43
5:O:224:TYR:HA	5:O:241:THR:HG23	2.00	0.43
1:A:215:LEU:HD22	1:A:261:VAL:HG22	1.99	0.43
5:E:141:GLU:O	5:E:144:ILE:HG12	2.18	0.43
4:N:141:LYS:HA	4:N:141:LYS:HE2	2.00	0.43
4:D:20:HIS:CE1	4:I:20:HIS:CE1	2.95	0.43
5:J:192:LEU:C	5:J:194:ASP:H	2.22	0.43
5:T:41:TRP:CD1	5:T:87:PHE:CE2	3.06	0.43
2:G:28:THR:HG23	2:G:63:TYR:HB3	2.00	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:E:58:ASP:O	5:E:59:VAL:C	2.56	0.43
1:A:5:MET:O	1:A:100:GLY:HA3	2.17	0.43
2:G:41:LYS:C	2:G:41:LYS:HD3	2.39	0.43
4:D:30:GLY:HA2	4:D:84(C):ARG:NH1	2.32	0.43
4:I:127:ILE:O	4:I:128:GLN:C	2.57	0.43
5:J:131:PRO:HA	5:J:223:PHE:CD2	2.53	0.43
5:T:7:MET:CB	5:T:8:PRO:CD	2.93	0.43
1:P:49:ALA:HB1	1:P:50:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:240:VAL:O	5:O:242:GLN:HG2	2.18	0.43
1:F:186:LYS:N	1:F:186:LYS:HD2	2.33	0.43
2:G:14:PRO:HA	2:G:15:PRO:HD3	1.70	0.43
1:A:7:TYR:CE1	3:C:2:SER:HB3	2.53	0.43
2:G:32:PRO:HB2	2:G:33:PRO:CD	2.48	0.43
2:Q:7:ILE:HB	2:Q:93:VAL:HG21	2.01	0.43
5:E:240:VAL:O	5:E:242:GLN:HG2	2.19	0.43
1:K:3:HIS:HA	1:K:29:ASP:OD1	2.18	0.43
4:I:134:VAL:O	4:I:134:VAL:HG13	2.18	0.43
4:N:3:LYS:CG	4:N:4:THR:H	2.31	0.43
5:T:243:ILE:HG12	5:T:243:ILE:O	2.19	0.43
5:O:80:ARG:HH21	5:O:84:ARG:HA	1.84	0.43
4:N:130:PRO:C	4:N:132:PRO:HD3	2.39	0.43
1:P:102:ASP:HB2	1:P:111:ARG:HB3	2.00	0.43
4:D:25:HIS:CD2	4:D:87:SER:HG	2.37	0.43
4:D:91:LEU:O	4:D:92:PRO:O	2.36	0.43
4:D:39:ILE:HG13	4:D:39:ILE:O	2.18	0.43
2:Q:28:THR:HG22	2:Q:63:TYR:HB2	2.01	0.43
1:A:81:LEU:HD21	3:C:10:VAL:HG11	2.01	0.43
5:J:44:GLN:HG3	5:J:49:GLY:C	2.39	0.43
4:D:46:PRO:O	4:D:47:LEU:CB	2.67	0.43
5:J:20:LEU:HD21	5:J:88:SER:HB3	1.99	0.43
1:A:66:LYS:NZ	3:C:1:SER:HB3	2.34	0.43
5:T:48:LEU:N	5:T:48:LEU:HD22	2.34	0.43
1:F:208:PHE:HE2	1:F:242:GLN:HA	1.84	0.43
1:F:147:TRP:HB3	1:F:152:ALA:HB3	2.01	0.43
4:N:81:LEU:C	4:N:81:LEU:HD12	2.39	0.43
5:J:25:GLN:HG3	5:J:26:ASP:N	2.34	0.43
4:D:170:THR:HG22	4:D:188:VAL:O	2.19	0.43
5:E:71:ILE:N	5:E:72:PRO:HD3	2.33	0.43
1:F:205:ALA:O	1:F:242:GLN:HA	2.19	0.43
1:P:5:MET:HE2	1:P:7:TYR:HE2	1.84	0.43
1:P:208:PHE:CE1	1:P:241:PHE:HB2	2.53	0.43
1:A:14:ARG:HB3	1:A:17:LEU:HD12	2.01	0.43
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
4:I:139:ASP:HB3	5:J:137:PHE:CE2	2.54	0.42
2:G:70:PHE:HD2	2:G:78:TYR:CZ	2.37	0.42
1:P:58:GLU:H	1:P:58:GLU:HG3	1.59	0.42
3:H:10:VAL:O	3:H:10:VAL:HG12	2.18	0.42
5:T:71:ILE:N	5:T:72:PRO:HD3	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:I:92:PRO:O	4:I:93:HIS:C	2.56	0.42
1:P:5:MET:HB2	1:P:168:LEU:HD13	2.01	0.42
1:K:180:LEU:H	1:K:180:LEU:HD13	1.85	0.42
4:D:175:LEU:O	4:D:175:LEU:HD12	2.19	0.42
5:T:91:LEU:HD22	5:T:98:GLN:NE2	2.33	0.42
5:T:81:LYS:HA	5:T:81:LYS:HD3	1.77	0.42
5:E:136:VAL:HG23	5:E:246:ALA:CB	2.49	0.42
5:E:44:GLN:HE21	5:E:44:GLN:HB2	1.61	0.42
1:A:225:THR:HG21	1:P:107:TRP:CE3	2.54	0.42
4:D:175:LEU:HB3	5:E:180:CYS:CB	2.41	0.42
5:J:77:ARG:NE	5:J:90:ILE:HG21	2.34	0.42
4:I:147:VAL:CG2	4:I:188:VAL:HG13	2.49	0.42
4:S:158:ASN:O	4:S:159:VAL:HG23	2.18	0.42
2:Q:49:VAL:HG22	2:Q:68:THR:HB	2.01	0.42
5:J:58:ASP:OD1	5:J:84:ARG:HD3	2.19	0.42
1:A:217:TRP:H	1:A:228:MET:CE	2.33	0.42
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
1:K:123:TYR:HH	1:K:143:THR:HG1	1.67	0.42
5:T:212:ASN:HB3	5:T:215:ASN:HB2	2.01	0.42
4:I:46:PRO:O	4:I:48:GLN:N	2.48	0.42
4:N:82:ALA:HB2	4:S:80:PHE:CE2	2.55	0.42
1:A:194:ARG:O	1:A:195:SER:HB3	2.19	0.42
1:K:272:LEU:O	1:K:272:LEU:HD12	2.20	0.42
5:T:192:LEU:N	5:T:192:LEU:HD12	2.35	0.42
5:J:77:ARG:NH2	5:J:90:ILE:HG21	2.34	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:T:132:PRO:O	5:T:133:GLU:C	2.57	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
5:J:205:VAL:HG11	5:J:209:PHE:CD2	2.54	0.42
2:Q:5:PRO:HD3	2:Q:86:SER:OG	2.19	0.42
5:T:50:LEU:H	5:T:50:LEU:HD12	1.84	0.42
1:A:44:ARG:HB2	1:A:64:THR:OG1	2.20	0.42
1:F:255:GLN:CD	1:F:255:GLN:H	2.22	0.42
4:I:178:ARG:H	4:I:179:SER:CB	2.31	0.42
5:T:160:TYR:HA	5:T:161:PRO:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.95	0.42
4:N:66:ASN:CG	4:N:67:THR:N	2.72	0.42
1:A:178:THR:C	1:A:180:LEU:H	2.23	0.42
1:F:210:PRO:HD3	1:F:264:GLU:OE2	2.19	0.42
4:D:127:ILE:HB	4:D:128:GLN:H	1.58	0.42
1:K:167:TRP:HB3	1:K:171:TYR:HE2	1.81	0.42
5:T:211:GLN:HE21	5:T:211:GLN:HA	1.85	0.42
5:T:20:LEU:HD11	5:T:88:SER:HB3	2.01	0.42
1:F:13:SER:O	1:F:92:SER:HA	2.20	0.42
2:B:39:MET:HB3	2:B:46:ILE:HD12	2.02	0.42
4:S:15:GLU:HB3	4:S:126:PRO:HA	2.01	0.42
2:B:85:ASP:OD1	2:B:85:ASP:N	2.53	0.42
4:N:95:SER:O	4:N:96:LEU:CB	2.67	0.41
5:O:2:MET:HE1	5:O:113:TYR:CE2	2.55	0.41
2:L:7:ILE:HD11	2:L:82:VAL:CG2	2.50	0.41
1:A:45:TYR:HE2	1:A:67:ALA:HB2	1.85	0.41
2:G:50:GLU:O	2:G:66:ALA:HA	2.20	0.41
1:F:61:GLU:O	1:F:65:GLN:HG2	2.20	0.41
4:I:155:SER:C	4:I:157:THR:H	2.23	0.41
5:T:224:TYR:HA	5:T:241:THR:HG23	2.02	0.41
5:J:30:GLU:HG3	5:J:84:ARG:HH21	1.84	0.41
4:S:5:THR:HG23	4:S:24:SER:HB2	2.02	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
1:F:201:LEU:O	1:F:246:SER:HA	2.21	0.41
4:S:14:THR:CG2	4:S:127:ILE:HG13	2.51	0.41
1:F:80:ASN:HA	1:P:86:ASN:ND2	2.35	0.41
4:I:137:LEU:N	4:I:137:LEU:HD12	2.35	0.41
4:S:44:GLN:HE22	5:T:50:LEU:HD11	1.84	0.41
2:Q:14:PRO:HA	2:Q:15:PRO:HD3	1.77	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
5:J:31:THR:HA	5:J:56:SER:O	2.20	0.41
5:T:151:THR:OG1	5:T:204:ARG:HD2	2.19	0.41
5:J:21:LEU:HB2	5:J:89:LEU:HB3	2.01	0.41
2:G:41:LYS:N	2:G:46:ILE:HD11	2.35	0.41
5:J:44:GLN:HB2	5:J:50:LEU:HD12	2.01	0.41
1:F:44:ARG:CZ	1:F:64:THR:HG21	2.51	0.41
4:D:25:HIS:O	4:D:25:HIS:ND1	2.51	0.41
1:F:74:PHE:HZ	1:F:97:GLN:HG2	1.85	0.41
1:F:8:PHE:HB3	2:G:56:PHE:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:125:ASP:OD1	5:T:127:LYS:HB2	2.20	0.41
1:K:209:TYR:C	1:K:209:TYR:HD2	2.22	0.41
1:A:209:TYR:C	1:A:209:TYR:CD2	2.94	0.41
5:T:44:GLN:HB2	5:T:50:LEU:HG	2.02	0.41
1:F:10:THR:O	1:F:22:TYR:HA	2.21	0.41
5:E:232:TRP:NE1	5:E:234:GLN:HB2	2.35	0.41
5:T:3:LYS:O	5:T:27:MET:HE1	2.20	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
5:T:143:GLU:CG	5:T:150:ALA:HB2	2.50	0.41
4:I:149:LEU:HD12	4:I:150:PHE:H	1.85	0.41
4:I:127:ILE:H	4:I:127:ILE:CD1	2.30	0.41
3:R:10:VAL:OXT	3:R:10:VAL:HG12	2.20	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
1:K:258:THR:HG22	1:K:273:ARG:HD3	2.03	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:D:84(C):ARG:O	4:D:85:LYS:HB2	2.21	0.41
4:I:32:GLU:HB3	4:I:108:GLY:HA2	2.02	0.41
1:F:273:ARG:HB3	1:F:274:TRP:H	1.54	0.41
4:N:28:ILE:HD11	4:N:32:GLU:HB2	2.03	0.41
1:F:98:MET:HE2	1:F:98:MET:HB3	1.98	0.41
2:B:23:LEU:HB2	2:B:70:PHE:CD1	2.56	0.41
4:I:183:LYS:O	4:I:184:SER:CB	2.69	0.41
5:T:151:THR:HB	5:T:203:LEU:O	2.21	0.41
5:O:59:VAL:HG12	5:O:60:ASP:N	2.34	0.41
5:O:232:TRP:HH2	5:O:236:ARG:NH1	2.18	0.41
1:A:147:TRP:HA	1:A:150:SER:HG	1.86	0.41
1:P:234:ARG:HG3	1:P:242:GLN:HG3	2.02	0.41
1:K:192:HIS:HB2	1:K:200:THR:O	2.20	0.41
1:K:181:ARG:HB3	1:K:181:ARG:CZ	2.51	0.41
1:A:225:THR:HB	1:P:107:TRP:CG	2.56	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
1:K:194:ARG:HD2	1:K:194:ARG:C	2.41	0.41
1:A:202:ARG:HD3	1:A:244:TRP:CD2	2.55	0.41
5:E:182:ASP:HB2	5:E:199:LEU:CD1	2.51	0.41
5:O:77:ARG:NH1	5:O:90:ILE:HD12	2.36	0.41
1:A:107:TRP:CE3	1:P:225:THR:HG22	2.56	0.41
1:P:184:SER:HA	1:P:185:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:181:THR:HG23	5:J:201:SER:HB2	2.01	0.41
5:O:66:ASN:ND2	5:O:78:VAL:HG23	2.25	0.41
1:K:8:PHE:HB3	2:L:56:PHE:CZ	2.56	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
4:N:82:ALA:HB2	4:S:80:PHE:CZ	2.56	0.41
5:J:39:MET:HA	5:J:105:ALA:O	2.21	0.41
1:K:209:TYR:HD2	1:K:210:PRO:N	2.19	0.41
5:T:187:LYS:HA	5:T:197:TYR:HA	2.03	0.41
5:T:96:THR:HG21	5:T:124:GLU:HG3	2.03	0.41
1:A:219:LEU:HD13	1:A:257:TYR:CZ	2.56	0.41
5:J:125:ASP:C	5:J:127:LYS:H	2.25	0.41
1:A:175:GLY:O	1:A:179:LEU:HG	2.21	0.41
1:K:78:LEU:O	1:K:82:LEU:HG	2.21	0.41
1:K:217:TRP:CE2	1:K:247:VAL:HG21	2.56	0.41
5:J:77:ARG:HE	5:J:90:ILE:HG21	1.85	0.40
4:N:191:SER:HA	4:N:192:ASN:HA	1.73	0.40
1:A:38:SER:O	1:A:43:PRO:HG3	2.22	0.40
4:I:137:LEU:HB3	5:J:138:GLU:O	2.21	0.40
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.56	0.40
1:A:160:LEU:O	1:A:164:CYS:HB3	2.21	0.40
1:A:25:VAL:HG12	1:A:27:TYR:CE1	2.56	0.40
1:K:259:CYS:O	1:K:271:THR:HG23	2.20	0.40
1:P:169:HIS:O	1:P:173:LYS:HG3	2.20	0.40
4:S:83:ILE:HD12	4:S:83:ILE:N	2.37	0.40
1:A:206:LEU:N	1:A:206:LEU:HD12	2.36	0.40
5:E:7:MET:O	5:E:8:PRO:C	2.57	0.40
5:J:202:ARG:HD2	5:J:202:ARG:N	2.35	0.40
1:P:72:GLN:HG3	1:P:75:ARG:HH22	1.87	0.40
2:B:7:ILE:HD11	2:B:82:VAL:HB	2.02	0.40
3:M:7:ARG:NH2	4:N:40:TYR:CE2	2.89	0.40
1:A:174:ASN:OD1	1:A:174:ASN:N	2.54	0.40
4:D:207:ILE:HG13	4:D:209:GLU:N	2.17	0.40
3:C:10:VAL:O	3:C:10:VAL:CG1	2.64	0.40
4:N:20:HIS:HE1	4:S:18:THR:OG1	2.03	0.40
2:Q:41:LYS:HB3	2:Q:78:TYR:CD2	2.56	0.40
5:J:17:GLU:HG2	5:J:18:ASN:H	1.86	0.40
5:J:56:SER:HB3	5:J:80:ARG:HH11	1.87	0.40
5:T:1:ASP:N	5:T:3:LYS:HE3	2.37	0.40
1:K:185:PRO:HA	1:K:207:GLY:O	2.21	0.40
1:A:147:TRP:HA	1:A:150:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:112:TYR:HB3	5:E:40:TYR:HH	1.86	0.40
5:E:220:GLN:HE21	5:E:243:ILE:HB	1.87	0.40
5:T:192:LEU:HD12	5:T:192:LEU:H	1.85	0.40
5:O:79:SER:HB3	5:O:88:SER:HB2	2.02	0.40
4:N:83:ILE:HG13	4:N:84:ALA:O	2.21	0.40
5:E:2:MET:HE2	5:E:113:TYR:CD1	2.56	0.40
1:F:72:GLN:HB3	1:F:72:GLN:HE21	1.54	0.40
5:E:77:ARG:CZ	5:E:90:ILE:HG21	2.52	0.40
2:L:71:THR:HA	2:L:72:PRO:HD3	1.85	0.40
2:G:22:ILE:HD13	2:G:69:GLU:HA	2.04	0.40
1:P:62:ARG:O	1:P:66:LYS:HG3	2.21	0.40
2:B:22:ILE:HD13	2:B:69:GLU:HA	2.04	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%)	17	62
1	F	263/275 (96%)	222 (84%)	39 (15%)	2 (1%)	24	69
1	K	273/275 (99%)	235 (86%)	30 (11%)	8 (3%)	6	36
1	P	271/275 (98%)	244 (90%)	25 (9%)	2 (1%)	26	72
2	B	96/99 (97%)	87 (91%)	7 (7%)	2 (2%)	9	46
2	G	96/99 (97%)	82 (85%)	11 (12%)	3 (3%)	5	34
2	L	96/99 (97%)	81 (84%)	13 (14%)	2 (2%)	9	46
2	Q	96/99 (97%)	87 (91%)	9 (9%)	0	100	100
3	C	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	2
3	H	8/10 (80%)	7 (88%)	1 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	8/10 (80%)	7 (88%)	0	1 (12%)	0	2
3	R	8/10 (80%)	7 (88%)	0	1 (12%)	0	2
4	D	183/195 (94%)	132 (72%)	37 (20%)	14 (8%)	1	8
4	I	184/195 (94%)	128 (70%)	45 (24%)	11 (6%)	2	16
4	N	170/195 (87%)	119 (70%)	40 (24%)	11 (6%)	1	13
4	S	168/195 (86%)	132 (79%)	31 (18%)	5 (3%)	5	35
5	E	238/240 (99%)	206 (87%)	24 (10%)	8 (3%)	5	31
5	J	238/240 (99%)	200 (84%)	30 (13%)	8 (3%)	5	31
5	O	238/240 (99%)	207 (87%)	25 (10%)	6 (2%)	7	41
5	T	238/240 (99%)	197 (83%)	34 (14%)	7 (3%)	6	36
All	All	3153/3276 (96%)	2629 (83%)	429 (14%)	95 (3%)	5	35

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	5	ASN
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	40 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	227/234 (97%)	220 (97%)	7 (3%)	47	82
1	K	234/234 (100%)	222 (95%)	12 (5%)	29	70
1	P	232/234 (99%)	222 (96%)	10 (4%)	35	75
2	B	93/94 (99%)	90 (97%)	3 (3%)	46	81
2	G	93/94 (99%)	86 (92%)	7 (8%)	17	55
2	L	93/94 (99%)	88 (95%)	5 (5%)	27	68
2	Q	93/94 (99%)	92 (99%)	1 (1%)	80	94
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%)	158 (94%)	11 (6%)	21	61
4	I	168/175 (96%)	150 (89%)	18 (11%)	8	34
4	N	154/175 (88%)	140 (91%)	14 (9%)	12	42
4	S	154/175 (88%)	140 (91%)	14 (9%)	12	42
5	E	213/213 (100%)	199 (93%)	14 (7%)	21	61
5	J	213/213 (100%)	199 (93%)	14 (7%)	21	61
5	O	213/213 (100%)	202 (95%)	11 (5%)	29	69
5	T	213/213 (100%)	197 (92%)	16 (8%)	17	55
All	All	2832/2900 (98%)	2666 (94%)	166 (6%)	24	65

All (166) 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	145	ARG
1	A	174	ASN
1	A	179	LEU
1	A	181	ARG
1	A	209	TYR
1	A	247	VAL
2	B	61	SER
2	B	85	ASP

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Mol	Chain	Res	Type
2	B	91	LYS
4	D	5	THR
4	D	11	MET
4	D	17	GLU
4	D	18	THR
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	17	GLU
5	E	31	THR
5	E	44	GLN
5	E	45	ASP
5	E	84	ARG
5	E	96	THR
5	E	157	THR
5	E	193	ASN
5	E	202	ARG
5	E	211	GLN
5	E	214	ARG
5	E	222	GLN
5	E	236	ARG
1	F	45	TYR
1	F	58	GLU
1	F	94	THR
1	F	122	ASP
1	F	179	LEU
1	F	230	LEU
1	F	255	GLN
2	G	28	THR
2	G	58	LYS
2	G	67	HIS
2	G	75	THR
2	G	81	ARG
2	G	85	ASP
2	G	92	THR
4	I	11	MET
4	I	18	THR

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Mol	Chain	Res	Type
4	I	31	ASN
4	I	39	ILE
4	I	43	ARG
4	I	45	VAL
4	I	47	LEU
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	14	ARG
5	J	31	THR
5	J	51	GLN
5	J	85	GLU
5	J	87	PHE
5	J	95	LYS
5	J	120	LEU
5	J	124	GLU
5	J	163	HIS
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	149	GLN
1	K	180	LEU
1	K	209	TYR
1	K	217	TRP
1	K	223	GLU
1	K	274	TRP

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Mol	Chain	Res	Type
2	L	2	GLN
2	L	8	GLN
2	L	38	GLN
2	L	70	PHE
2	L	91	LYS
4	N	12	GLU
4	N	18	THR
4	N	31	ASN
4	N	47	LEU
4	N	59	GLN
4	N	69	ASN
4	N	78	MET
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
5	O	90	ILE
5	O	111	GLU
5	O	146	HIS
5	O	163	HIS
5	O	192	LEU
5	O	236	ARG
1	P	9	GLU
1	P	17	LEU
1	P	22	TYR
1	P	58	GLU
1	P	107	TRP
1	P	109	LEU
1	P	143	THR
1	P	145	ARG
1	P	260	ARG
1	P	270	LEU
2	Q	67	HIS
4	S	5	THR

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Mol	Chain	Res	Type
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	178	ARG
4	S	183	LYS
4	S	196	PHE
5	T	12	ILE
5	T	19	VAL
5	T	25	GLN
5	T	54	TYR
5	T	90	ILE
5	T	91	LEU
5	T	146	HIS
5	T	152	LEU
5	T	193	ASN
5	T	194	ASP
5	T	202	ARG
5	T	211	GLN
5	T	212	ASN
5	T	236	ARG
5	T	243	ILE
5	T	251	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	87	GLN
1	A	96	GLN
1	A	127	ASN
1	A	169	HIS
1	A	191	HIS
1	A	226	GLN
1	A	263	HIS
2	B	2	GLN

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Mol	Chain	Res	Type
2	B	31	HIS
4	D	20	HIS
4	D	44	GLN
4	D	136	GLN
4	D	185	ASN
4	D	204	ASN
5	E	18	ASN
5	E	29	HIS
5	E	44	GLN
5	E	146	HIS
5	E	171	ASN
5	E	216	HIS
5	E	220	GLN
5	E	242	GLN
1	F	65	GLN
1	F	72	GLN
1	F	87	GLN
1	F	96	GLN
1	F	149	GLN
1	F	169	HIS
1	F	218	GLN
1	F	255	GLN
2	G	8	GLN
2	G	67	HIS
4	I	20	HIS
4	I	66	ASN
4	I	111	ASN
4	I	128	GLN
4	I	158	ASN
5	J	6	GLN
5	J	18	ASN
5	J	146	HIS
5	J	171	ASN
5	J	216	HIS
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

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Mol	Chain	Res	Type
4	N	25	HIS
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	163	HIS
5	O	216	HIS
5	O	242	GLN
1	P	54	GLN
1	P	65	GLN
1	P	87	GLN
1	P	96	GLN
1	P	169	HIS
1	P	176	ASN
1	P	263	HIS
2	Q	2	GLN
2	Q	8	GLN
2	Q	17	ASN
2	Q	31	HIS
3	R	5	ASN
4	S	20	HIS
4	S	31	ASN
4	S	44	GLN
4	S	59	GLN
4	S	66	ASN
4	S	128	GLN
4	S	156	GLN
5	T	6	GLN
5	T	29	HIS
5	T	98	GLN
5	T	171	ASN
5	T	193	ASN
5	T	211	GLN
5	T	234	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	0.21	9 (3%) 50 35	27, 74, 122, 148	1 (0%)
1	F	267/275 (97%)	0.48	23 (8%) 13 7	37, 100, 168, 201	1 (0%)
1	K	275/275 (100%)	0.54	26 (9%) 10 6	29, 95, 177, 194	0
1	P	273/275 (99%)	0.47	18 (6%) 22 12	38, 90, 152, 165	1 (0%)
2	B	98/99 (98%)	0.01	0 100 100	42, 68, 103, 112	0
2	G	98/99 (98%)	0.32	3 (3%) 52 38	54, 104, 152, 156	0
2	L	98/99 (98%)	0.33	2 (2%) 68 54	53, 100, 144, 151	0
2	Q	98/99 (98%)	0.35	3 (3%) 52 38	58, 97, 129, 145	0
3	C	10/10 (100%)	-0.04	1 (10%) 9 5	31, 38, 66, 70	0
3	H	10/10 (100%)	-0.06	0 100 100	40, 49, 81, 88	0
3	M	10/10 (100%)	0.05	0 100 100	37, 44, 71, 83	0
3	R	10/10 (100%)	0.20	1 (10%) 9 5	42, 49, 80, 86	0
4	D	189/195 (96%)	0.36	4 (2%) 67 52	32, 79, 149, 169	0
4	I	188/195 (96%)	0.24	4 (2%) 67 52	40, 85, 146, 163	0
4	N	174/195 (89%)	0.45	12 (6%) 20 11	37, 79, 162, 179	0
4	S	174/195 (89%)	0.37	6 (3%) 49 34	40, 85, 150, 197	0
5	E	240/240 (100%)	0.06	2 (0%) 87 80	32, 69, 120, 135	0
5	J	240/240 (100%)	0.10	8 (3%) 50 35	32, 69, 128, 152	0
5	O	240/240 (100%)	0.14	2 (0%) 87 80	31, 69, 113, 149	0
5	T	240/240 (100%)	0.28	1 (0%) 93 90	40, 90, 135, 155	0
All	All	3207/3276 (97%)	0.30	125 (3%) 43 28	27, 82, 152, 201	3 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	179	LEU	5.7
1	F	180	LEU	5.3
1	K	223	GLU	5.2
1	K	215	LEU	4.9
1	K	222	GLU	4.8
4	D	213	PHE	4.8
4	N	182	PHE	4.4
4	N	180	MET	4.4
4	N	179	SER	4.2
1	F	185	PRO	4.2
4	N	142	SER	4.2
1	P	221	GLY	4.1
1	P	217	TRP	4.1
1	K	193	PRO	3.9
1	P	270	LEU	3.9
2	Q	78	TYR	3.8
4	S	182	PHE	3.7
1	K	220	ASN	3.7
1	P	249	VAL	3.7
1	F	205	ALA	3.7
1	F	196	LYS	3.6
1	A	225	THR	3.5
1	F	264	GLU	3.5
1	A	105	SER	3.5
4	D	180	MET	3.5
1	F	189	VAL	3.5
4	N	128	GLN	3.4
1	P	247	VAL	3.4
5	E	193	ASN	3.4
1	P	177	ALA	3.4
1	A	220	ASN	3.3
1	K	247	VAL	3.2
1	K	224	LEU	3.2
4	S	180	MET	3.2
1	K	105	SER	3.2
2	L	15	PRO	3.2
1	P	201	LEU	3.1
1	K	217	TRP	3.1
1	F	256	ASN	3.1
1	F	178	THR	3.1
1	K	201	LEU	3.1
1	K	216	THR	3.0
1	K	104	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	176	ASN	3.0
5	O	253	ASP	3.0
1	F	105	SER	2.9
5	T	147	THR	2.9
2	G	15	PRO	2.8
1	P	250	PRO	2.8
1	P	272	LEU	2.8
1	K	197	GLY	2.8
5	J	141	GLU	2.7
1	F	250	PRO	2.7
1	F	184	SER	2.7
1	P	225	THR	2.7
1	F	273	ARG	2.6
1	P	271	THR	2.6
1	F	183	ASP	2.6
1	F	197	GLY	2.6
1	K	196	LYS	2.6
1	F	177	ALA	2.6
1	K	256	ASN	2.6
1	K	257	TYR	2.6
3	R	1	SER	2.6
1	A	180	LEU	2.6
1	F	251	LEU	2.5
1	K	260	ARG	2.5
1	P	222	GLU	2.5
5	J	150	ALA	2.5
2	G	77	THR	2.5
1	F	254	GLU	2.5
1	F	104	GLY	2.5
4	N	129	ASN	2.5
1	K	221	GLY	2.4
4	I	144	ASP	2.4
4	S	157	THR	2.4
1	F	262	TYR	2.4
4	S	190	TRP	2.4
1	K	225	THR	2.4
4	N	181	ASP	2.4
1	P	257	TYR	2.4
2	Q	47	PRO	2.4
4	N	177	MET	2.4
1	K	253	LYS	2.3
4	D	202	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLY	2.3
4	N	188	VAL	2.3
4	N	176	ASP	2.3
5	J	248	ALA	2.3
4	S	178	ARG	2.3
4	I	205	SER	2.3
2	G	23	LEU	2.2
2	L	22	ILE	2.2
1	K	219	LEU	2.2
2	Q	15	PRO	2.2
1	A	273	ARG	2.2
1	K	228	MET	2.2
1	A	223	GLU	2.2
4	D	199	ALA	2.2
5	O	193	ASN	2.2
1	P	259	CYS	2.2
1	K	246	SER	2.2
1	F	190	THR	2.2
1	F	186	LYS	2.1
4	N	178	ARG	2.1
1	A	196	LYS	2.1
5	J	149	LYS	2.1
1	P	223	GLU	2.1
1	K	276	PRO	2.1
4	N	78	MET	2.1
4	I	196	PHE	2.1
1	K	205	ALA	2.1
1	F	242	GLN	2.1
1	P	224	LEU	2.1
4	I	198	CYS	2.1
1	K	175	GLY	2.1
3	C	1	SER	2.0
5	E	232	TRP	2.0
5	J	143	GLU	2.0
1	P	176	ASN	2.0
5	J	193	ASN	2.0
5	J	251	ARG	2.0
1	P	183	ASP	2.0
4	S	151	THR	2.0
5	J	155	LEU	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 carbohydrates 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.