



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2023 – 01:37 AM EDT

PDB ID : 2IAN  
Title : Structural basis for recognition of mutant self by a tumor-specific, MHC class II-restricted TCR  
Authors : Deng, L.; Langley, R.J.; Mariuzza, R.A.  
Deposited on : 2006-09-08  
Resolution : 2.80 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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

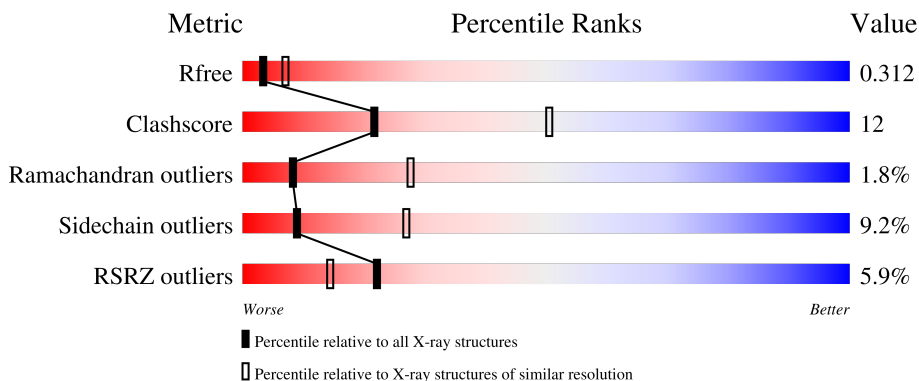
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	182	 3% 66% 25% 7%
1	F	182	 5% 70% 25%
1	K	182	 18% 69% 25%
1	P	182	 10% 74% 23%
2	B	190	 6% 63% 28% 5%

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Mol	Chain	Length	Quality of chain
2	G	190	4% 67% 24% . .
2	L	190	% 72% 23% 5% .
2	Q	190	2% 67% 26% 5% ..
3	C	15	73% 20% 7%
3	H	15	7% 53% 33% 13%
3	M	15	7% 60% 20% 13% 7%
3	R	15	73% 20% 7%
4	D	202	6% 69% 24% 5% .
4	I	202	7% 65% 27% 5% .
4	N	202	11% 64% 29% . . .
4	S	202	16% 63% 29% 5% ..
5	E	240	78% 18% . .
5	J	240	% 69% 27% .
5	O	240	2% 70% 26% . . .
5	T	240	3% 68% 27% . .

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26209 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	178	1464	949	238	272	5	0	0	0
1	F	179	1473	954	239	275	5	0	0	0
1	K	179	1473	954	239	275	5	0	0	0
1	P	179	1473	954	239	275	5	0	0	0

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	181	1485	936	265	278	6	0	0	0
2	G	182	1493	940	266	281	6	0	0	0
2	L	188	1544	973	277	288	6	0	0	0
2	Q	188	1544	973	277	288	6	0	0	0

- Molecule 3 is a protein called 15-mer peptide from Triosephosphate isomerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	15	103	64	17	22	0	0	0
3	H	15	103	64	17	22	0	0	0
3	M	15	103	64	17	22	0	0	0
3	R	15	103	64	17	22	0	0	0

- Molecule 4 is a protein called CD4+ T cell receptor E8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	198	Total	C	N	O	S	0	0	0
			1546	967	260	312	7			
4	I	198	Total	C	N	O	S	0	0	0
			1546	967	260	312	7			
4	N	198	Total	C	N	O	S	0	0	0
			1546	967	260	312	7			
4	S	198	Total	C	N	O	S	0	0	0
			1546	967	260	312	7			

- Molecule 5 is a protein called CD4+ T cell receptor E8 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	238	Total	C	N	O	S	0	0	0
			1896	1203	323	361	9			
5	J	239	Total	C	N	O	S	0	0	0
			1901	1206	324	362	9			
5	O	238	Total	C	N	O	S	0	0	0
			1895	1203	323	360	9			
5	T	238	Total	C	N	O	S	0	0	0
			1896	1203	323	361	9			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	8	Total	O	0	0
			8	8		
6	D	6	Total	O	0	0
			6	6		
6	E	6	Total	O	0	0
			6	6		
6	F	5	Total	O	0	0
			5	5		
6	G	10	Total	O	0	0
			10	10		
6	I	6	Total	O	0	0
			6	6		
6	J	10	Total	O	0	0
			10	10		
6	L	4	Total	O	0	0
			4	4		

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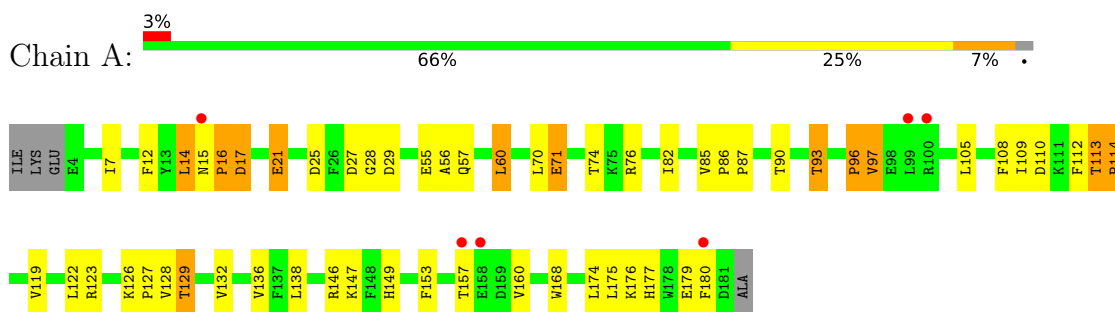
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
6	N	4	Total O 4 4	0	0
6	O	1	Total O 1 1	0	0
6	P	2	Total O 2 2	0	0
6	Q	2	Total O 2 2	0	0
6	S	2	Total O 2 2	0	0
6	T	6	Total O 6 6	0	0

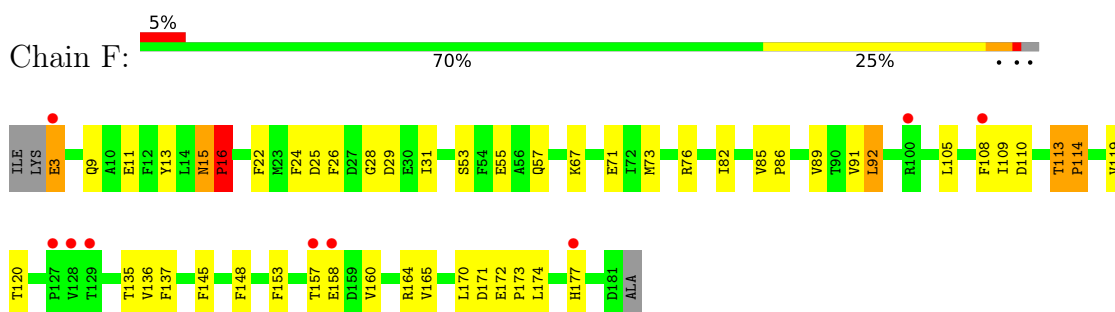
### 3 Residue-property plots

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

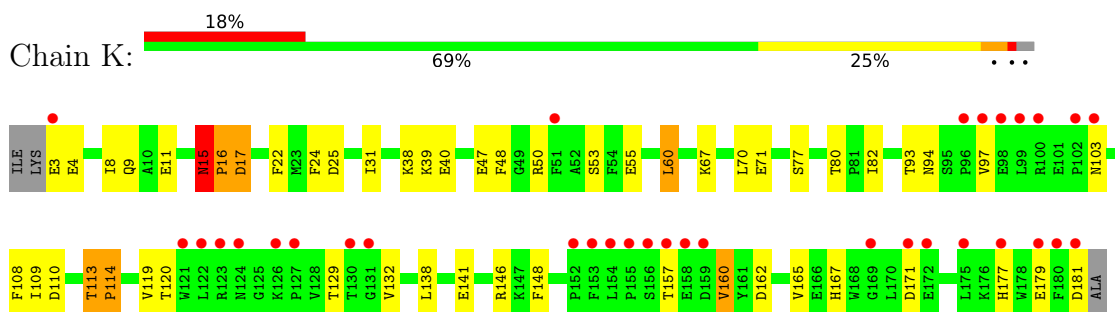
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



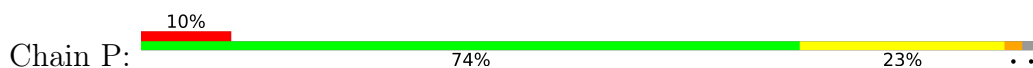
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

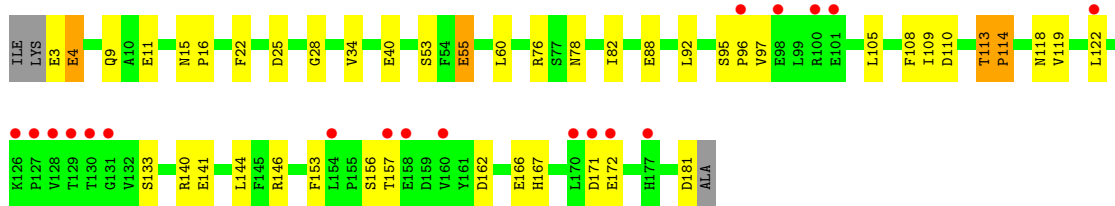


- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

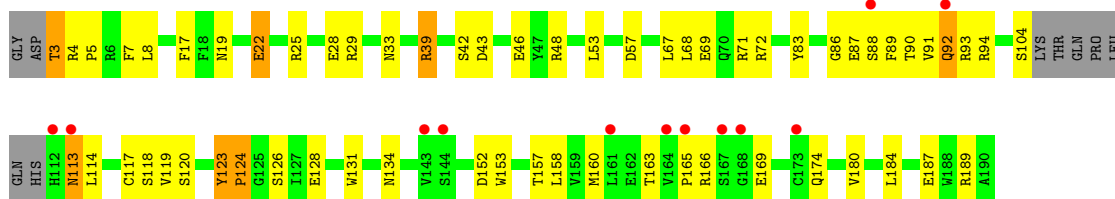


- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

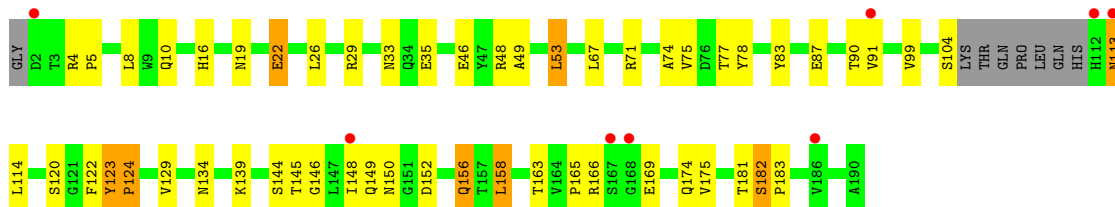




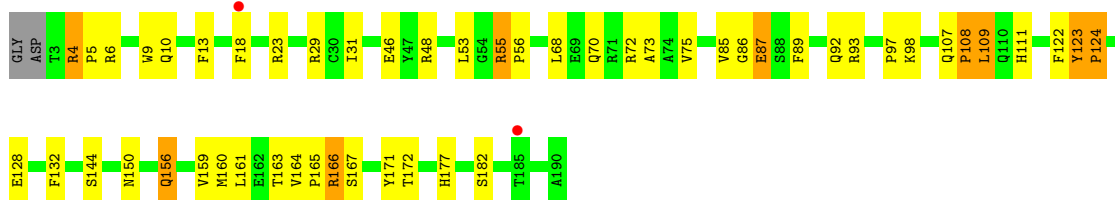
● Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain



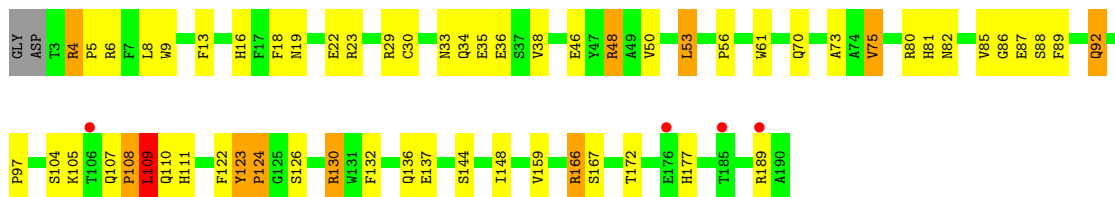
● Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain



● Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

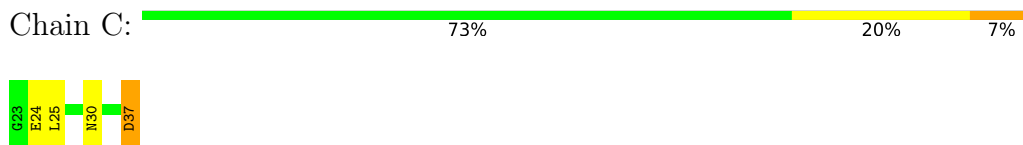


● Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain





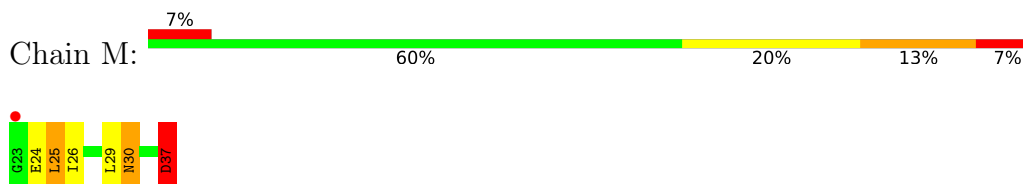
- Molecule 3: 15-mer peptide from Triosephosphate isomerase



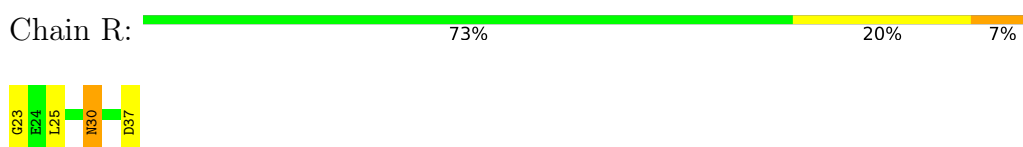
- Molecule 3: 15-mer peptide from Triosephosphate isomerase



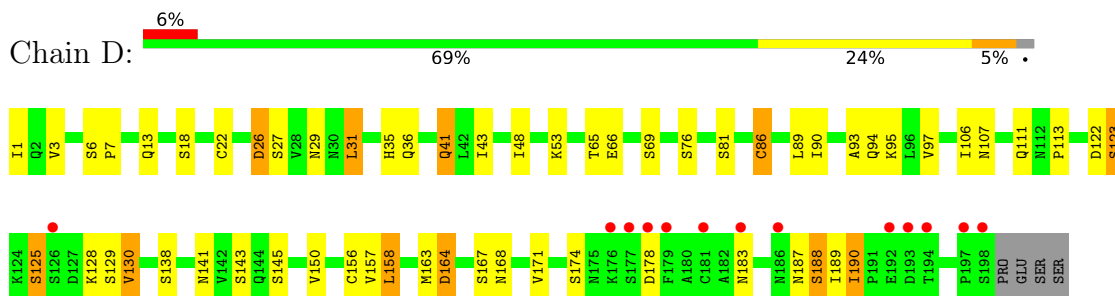
- Molecule 3: 15-mer peptide from Triosephosphate isomerase



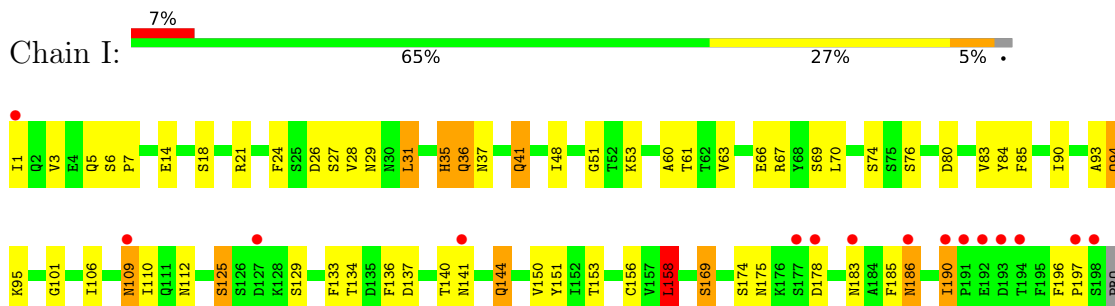
- Molecule 3: 15-mer peptide from Triosephosphate isomerase



- Molecule 4: CD4+ T cell receptor E8 alpha chain

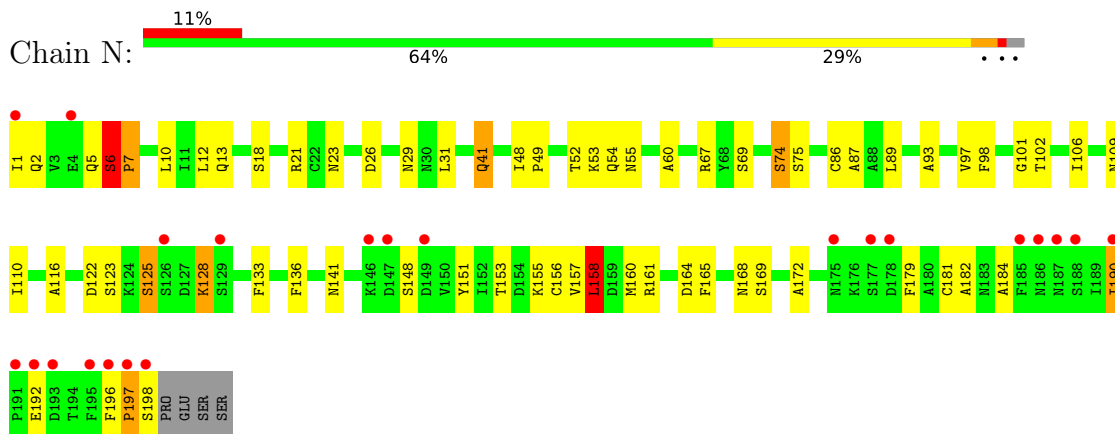


- Molecule 4: CD4+ T cell receptor E8 alpha chain

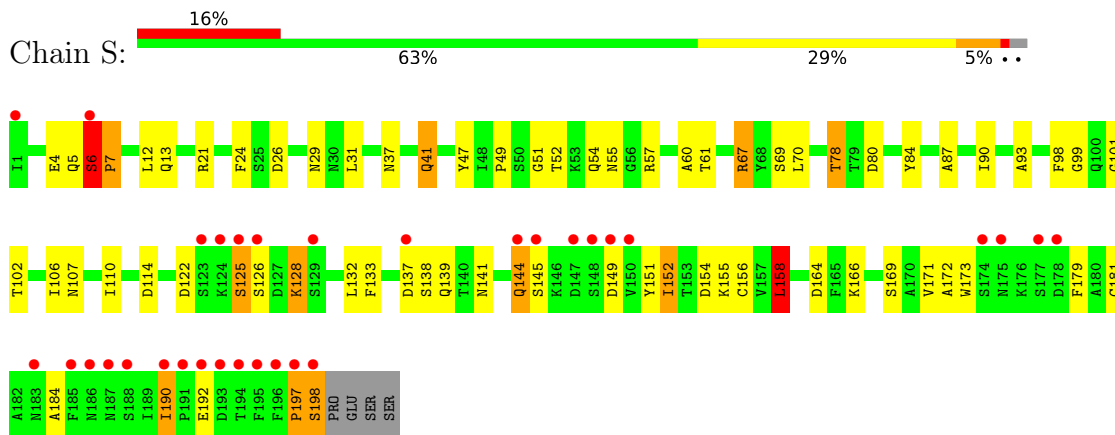


GLU  
SER  
SER

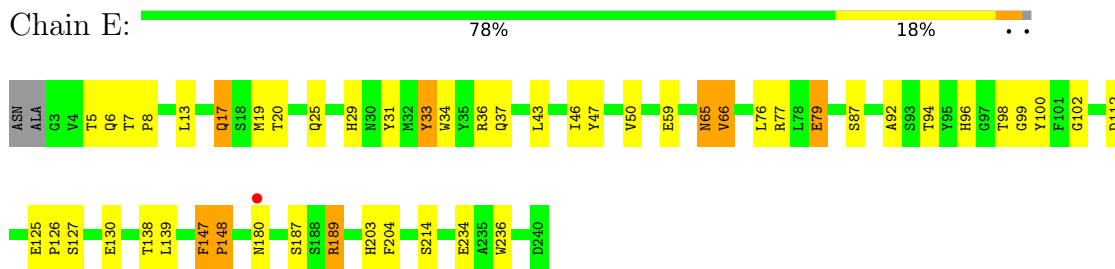
• Molecule 4: CD4+ T cell receptor E8 alpha chain



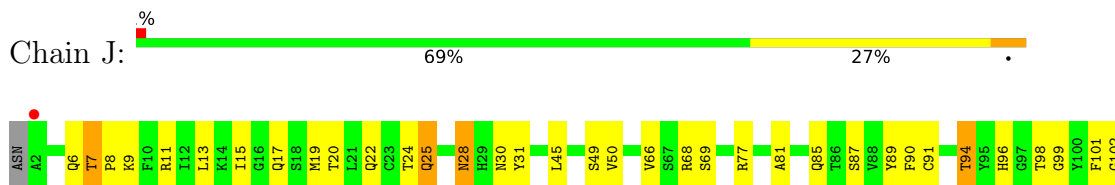
• Molecule 4: CD4+ T cell receptor E8 alpha chain

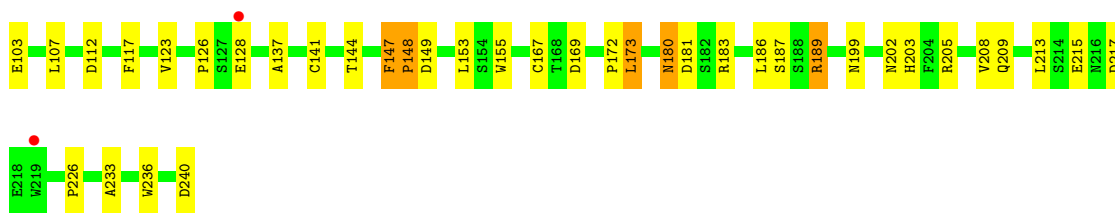


• Molecule 5: CD4+ T cell receptor E8 beta chain

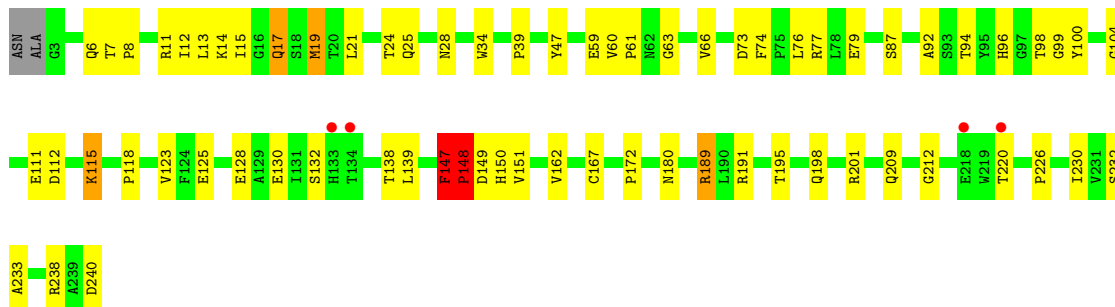


• Molecule 5: CD4+ T cell receptor E8 beta chain

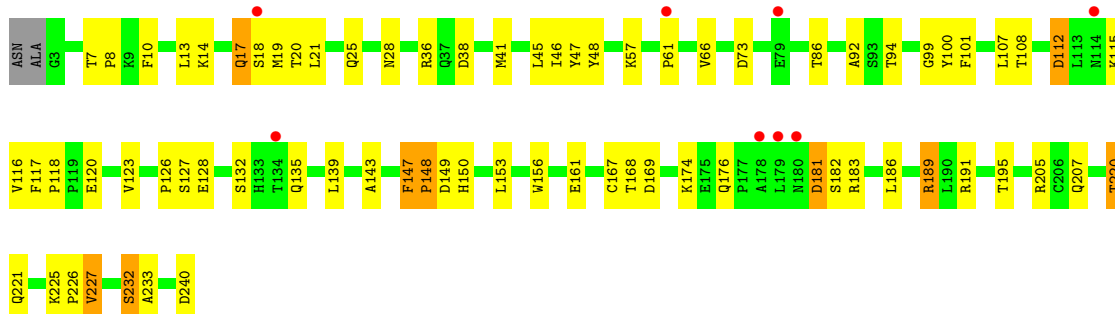




• Molecule 5: CD4+ T cell receptor E8 beta chain



• Molecule 5: CD4+ T cell receptor E8 beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.47Å 242.87Å 105.22Å 90.00° 111.32° 90.00°	Depositor
Resolution (Å)	45.45 – 2.80 45.45 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (45.45-2.80) 93.8 (45.45-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.221 , 0.296 0.253 , 0.312	Depositor DCC
$R_{free}$ test set	5054 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtrriage
Anisotropy	0.509	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 18.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	26209	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.19 % 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 6.0021e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.59	0/1509	0.71	0/2058
1	F	0.62	0/1518	0.73	0/2070
1	K	0.54	0/1518	0.69	1/2070 (0.0%)
1	P	0.57	0/1518	0.69	0/2070
2	B	0.67	0/1522	0.79	3/2066 (0.1%)
2	G	0.67	0/1530	0.79	1/2077 (0.0%)
2	L	0.59	0/1584	0.72	0/2152
2	Q	0.61	0/1584	0.71	1/2152 (0.0%)
3	C	0.82	0/103	0.98	0/138
3	H	0.76	0/103	0.95	0/138
3	M	0.71	0/103	0.97	1/138 (0.7%)
3	R	0.73	0/103	0.78	0/138
4	D	0.63	0/1579	0.78	1/2148 (0.0%)
4	I	0.65	0/1579	0.82	3/2148 (0.1%)
4	N	0.62	1/1579 (0.1%)	0.75	1/2148 (0.0%)
4	S	0.61	0/1579	0.74	1/2148 (0.0%)
5	E	0.67	0/1951	0.75	0/2659
5	J	0.68	1/1956 (0.1%)	0.75	1/2666 (0.0%)
5	O	0.60	0/1950	0.69	1/2658 (0.0%)
5	T	0.60	0/1951	0.68	0/2659
All	All	0.63	2/26819 (0.0%)	0.74	15/36501 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	F	0	2
1	K	0	2
1	P	0	2
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1
2	L	0	1
2	Q	0	1
4	D	0	1
4	I	0	1
4	N	0	1
4	S	0	1
5	E	0	2
5	J	0	2
5	O	0	2
5	T	0	2
All	All	0	24

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	215	GLU	CB-CG	5.20	1.62	1.52
4	N	86	CYS	CB-SG	-5.03	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	15	ASN	C-N-CD	-6.80	105.64	120.60
4	I	158	LEU	CA-CB-CG	6.76	130.84	115.30
5	O	147	PHE	C-N-CD	-6.64	106.00	120.60
4	D	31	LEU	CA-CB-CG	-6.41	100.56	115.30
4	N	158	LEU	CA-CB-CG	6.39	130.00	115.30
3	M	37	ASP	CB-CG-OD2	5.96	123.67	118.30
2	Q	123	TYR	C-N-CD	-5.71	108.05	120.60
4	I	35	HIS	CA-C-N	5.53	129.37	117.20
4	S	158	LEU	CA-CB-CG	5.28	127.45	115.30
2	B	94	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	G	158	LEU	CA-CB-CG	5.13	127.10	115.30
2	B	39	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	B	72	ARG	NE-CZ-NH2	-5.05	117.77	120.30
5	J	45	LEU	CA-CB-CG	5.04	126.89	115.30
4	I	35	HIS	O-C-N	-5.02	114.66	122.70

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	THR	Peptide
1	A	14	LEU	Peptide
2	B	123	TYR	Peptide
4	D	6	SER	Peptide
5	E	147	PHE	Peptide
5	E	7	THR	Peptide
1	F	113	THR	Peptide
1	F	15	ASN	Peptide
2	G	123	TYR	Peptide
4	I	6	SER	Peptide
5	J	147	PHE	Peptide
5	J	7	THR	Peptide
1	K	113	THR	Peptide
1	K	15	ASN	Peptide
2	L	123	TYR	Peptide
4	N	6	SER	Peptide
5	O	147	PHE	Peptide
5	O	7	THR	Peptide
1	P	113	THR	Peptide
1	P	15	ASN	Peptide
2	Q	123	TYR	Peptide
4	S	6	SER	Peptide
5	T	147	PHE	Peptide
5	T	7	THR	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1464	0	1401	47	1
1	F	1473	0	1407	38	0
1	K	1473	0	1407	32	1
1	P	1473	0	1407	29	0
2	B	1485	0	1416	43	0
2	G	1493	0	1420	38	0
2	L	1544	0	1478	39	0
2	Q	1544	0	1478	50	0
3	C	103	0	105	2	0
3	H	103	0	105	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	103	0	105	7	0
3	R	103	0	105	3	0
4	D	1546	0	1474	36	0
4	I	1546	0	1474	43	0
4	N	1546	0	1474	58	0
4	S	1546	0	1474	57	0
5	E	1896	0	1795	33	0
5	J	1901	0	1800	44	0
5	O	1895	0	1795	37	0
5	T	1896	0	1795	42	0
6	A	4	0	0	0	0
6	B	8	0	0	1	0
6	D	6	0	0	0	0
6	E	6	0	0	0	0
6	F	5	0	0	1	0
6	G	10	0	0	0	0
6	I	6	0	0	0	0
6	J	10	0	0	0	0
6	L	4	0	0	0	0
6	N	4	0	0	0	0
6	O	1	0	0	0	0
6	P	2	0	0	0	0
6	Q	2	0	0	0	0
6	S	2	0	0	0	0
6	T	6	0	0	0	0
All	All	26209	0	24915	608	1

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 12.

All (608) 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)
1:A:82:ILE:HD13	1:A:114:PRO:HD3	1.23	1.12
2:Q:124:PRO:HD2	2:Q:177:HIS:HE2	1.15	1.09
1:F:55:GLU:HG2	4:I:93:ALA:HB2	1.38	1.05
2:Q:124:PRO:HD2	2:Q:177:HIS:NE2	1.75	1.01
4:D:1:ILE:N	4:D:27:SER:HB2	1.75	1.00
2:G:4:ARG:HB2	2:G:5:PRO:HD2	1.44	1.00
4:D:48:ILE:HD13	4:D:53:LYS:HB2	1.45	0.97
5:T:94:THR:HG22	5:T:99:GLY:HA2	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:NE1	2:B:3:THR:HG21	1.83	0.93
4:I:36:GLN:HA	4:I:41:GLN:O	1.70	0.92
4:I:41:GLN:OE1	5:J:103:GLU:HG2	1.71	0.89
4:D:1:ILE:H1	4:D:27:SER:HB2	1.39	0.86
2:L:55:ARG:HG3	2:L:55:ARG:HH11	1.39	0.85
5:E:94:THR:CG2	5:E:99:GLY:HA2	2.06	0.85
4:N:31:LEU:HD22	4:N:69:SER:HB2	1.59	0.85
2:B:4:ARG:HB2	2:B:5:PRO:HD2	1.56	0.84
5:E:94:THR:HG22	5:E:99:GLY:HA2	1.58	0.84
4:N:31:LEU:CD2	4:N:69:SER:CB	2.55	0.84
1:F:82:ILE:HD13	1:F:114:PRO:HD3	1.57	0.84
2:Q:124:PRO:CD	2:Q:177:HIS:HE2	1.91	0.84
2:Q:46:GLU:OE2	2:Q:48:ARG:NH1	2.11	0.83
5:E:65:ASN:ND2	5:E:66:VAL:H	1.77	0.82
1:K:16:PRO:HD2	1:K:17:ASP:OD1	1.81	0.81
5:J:169:ASP:HB2	5:J:186:LEU:CD1	2.12	0.80
5:E:147:PHE:CD2	5:E:148:PRO:HD3	2.17	0.79
2:Q:124:PRO:CD	2:Q:177:HIS:NE2	2.45	0.79
1:P:82:ILE:HD13	1:P:114:PRO:HD3	1.62	0.79
5:E:65:ASN:HD22	5:E:66:VAL:H	1.27	0.79
5:T:147:PHE:CD2	5:T:148:PRO:HD3	2.18	0.79
4:S:31:LEU:HD13	4:S:69:SER:HB2	1.63	0.79
2:G:4:ARG:HB2	2:G:5:PRO:CD	2.14	0.78
1:K:82:ILE:HD13	1:K:114:PRO:HD3	1.66	0.78
5:J:169:ASP:HB2	5:J:186:LEU:HD12	1.66	0.77
2:G:46:GLU:OE2	2:G:48:ARG:NH2	2.18	0.77
4:N:158:LEU:HD11	5:O:191:ARG:HB2	1.67	0.77
2:L:163:THR:HG21	2:L:171:TYR:OH	1.84	0.77
4:N:31:LEU:CD2	4:N:69:SER:HB3	2.14	0.75
4:I:94:GLN:HE21	4:I:94:GLN:HA	1.50	0.75
5:O:123:VAL:HG23	5:O:233:ALA:HB3	1.69	0.75
1:F:13:TYR:CE2	1:F:67:LYS:HG3	2.24	0.73
4:N:6:SER:HB3	4:N:7:PRO:HD2	1.72	0.72
4:N:122:ASP:HB2	4:N:128:LYS:HB2	1.71	0.72
4:S:122:ASP:HB2	4:S:128:LYS:HB2	1.70	0.72
4:I:144:GLN:HA	4:I:144:GLN:HE21	1.54	0.71
1:A:55:GLU:HG2	4:D:93:ALA:HB2	1.70	0.71
3:C:24:GLU:OE1	4:D:26:ASP:HB2	1.90	0.71
1:K:9:GLN:HB3	2:L:13:PHE:HB2	1.72	0.71
1:A:129:THR:O	1:A:132:VAL:HG22	1.91	0.70
5:T:86:THR:HG23	5:T:108:THR:HA	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:31:LEU:CD1	4:S:69:SER:HB2	2.22	0.70
5:E:65:ASN:HD22	5:E:66:VAL:N	1.89	0.70
4:D:1:ILE:H1	4:D:27:SER:CB	2.04	0.70
4:I:63:VAL:O	4:I:66:GLU:O	2.10	0.69
2:G:8:LEU:H	2:G:33:ASN:ND2	1.90	0.69
4:N:21:ARG:HG2	4:N:23:ASN:OD1	1.91	0.69
1:A:93:THR:HG21	1:A:97:VAL:HG22	1.75	0.69
2:B:69:GLU:OE2	4:D:53:LYS:HD2	1.91	0.69
4:N:41:GLN:HE21	4:N:41:GLN:HA	1.58	0.69
1:F:105:LEU:HG	1:F:153:PHE:CE1	2.28	0.68
2:L:10:GLN:HB2	2:L:31:ILE:HB	1.75	0.68
4:D:158:LEU:C	4:D:158:LEU:HD23	2.13	0.68
5:J:7:THR:OG1	5:J:22:GLN:HB2	1.94	0.68
4:D:48:ILE:CD1	4:D:53:LYS:HB2	2.22	0.68
2:Q:38:VAL:HG11	2:Q:61:TRP:HZ3	1.58	0.67
5:J:147:PHE:CD2	5:J:148:PRO:HD3	2.29	0.67
4:S:31:LEU:HD13	4:S:69:SER:CB	2.24	0.67
2:G:163:THR:O	2:G:165:PRO:HD3	1.95	0.67
5:T:220:THR:HG22	5:T:221:GLN:HE21	1.59	0.67
4:N:54:GLN:HG2	4:N:55:ASN:N	2.10	0.67
4:I:35:HIS:CD2	4:I:36:GLN:O	2.49	0.67
4:S:144:GLN:HA	4:S:144:GLN:NE2	2.10	0.66
4:S:169:SER:OG	5:T:189:ARG:CD	2.44	0.66
1:K:16:PRO:HD2	1:K:17:ASP:H	1.60	0.66
5:J:94:THR:HG23	5:J:99:GLY:HA2	1.77	0.66
2:B:90:THR:OG1	2:B:91:VAL:N	2.27	0.65
4:S:151:TYR:O	4:S:172:ALA:HA	1.96	0.65
5:O:94:THR:CG2	5:O:99:GLY:HA2	2.26	0.65
5:E:94:THR:HG22	5:E:99:GLY:CA	2.27	0.65
4:S:47:TYR:CZ	4:S:49:PRO:HG3	2.32	0.65
5:O:147:PHE:CD2	5:O:148:PRO:HD3	2.32	0.64
5:E:94:THR:HG22	5:E:98:THR:O	1.98	0.64
1:F:55:GLU:CG	4:I:93:ALA:HB2	2.22	0.64
2:G:139:LYS:HE2	2:G:139:LYS:HA	1.80	0.64
5:J:94:THR:HG22	5:J:98:THR:O	1.97	0.64
1:P:105:LEU:HG	1:P:153:PHE:CE1	2.33	0.63
4:N:31:LEU:CD2	4:N:69:SER:HB2	2.22	0.63
5:T:94:THR:CG2	5:T:99:GLY:HA2	2.24	0.63
1:K:119:VAL:HG22	1:K:165:VAL:HG22	1.81	0.63
5:T:116:VAL:HA	5:T:148:PRO:HD2	1.80	0.63
4:S:7:PRO:O	4:S:102:THR:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:31:LEU:HD21	4:N:69:SER:HB3	1.81	0.63
5:O:59:GLU:O	5:O:61:PRO:HD3	1.99	0.63
4:S:169:SER:OG	5:T:189:ARG:HD3	1.99	0.63
4:I:26:ASP:OD1	4:I:67:ARG:NH1	2.32	0.63
2:Q:124:PRO:HD3	2:Q:177:HIS:CE1	2.33	0.63
5:E:147:PHE:CD2	5:E:148:PRO:CD	2.81	0.62
2:B:4:ARG:HB2	2:B:5:PRO:CD	2.29	0.62
1:A:168:TRP:CE2	2:B:3:THR:HG21	2.33	0.62
1:F:76:ARG:HD2	2:G:53:LEU:HD23	1.80	0.62
2:G:104:SER:HB3	2:G:114:LEU:HB3	1.82	0.62
5:E:6:GLN:HE21	5:E:102:GLY:HA3	1.63	0.62
5:O:94:THR:HG22	5:O:98:THR:O	1.99	0.62
4:N:155:LYS:HA	4:N:169:SER:O	1.98	0.62
1:P:141:GLU:OE2	2:Q:29:ARG:NH2	2.33	0.61
5:E:94:THR:CG2	5:E:99:GLY:CA	2.78	0.61
2:L:150:ASN:HD21	2:L:156:GLN:HG2	1.65	0.61
2:L:46:GLU:OE2	2:L:48:ARG:NH1	2.32	0.61
1:P:95:SER:HB2	1:P:96:PRO:HD2	1.82	0.61
1:A:82:ILE:CD1	1:A:114:PRO:HD3	2.15	0.61
4:D:1:ILE:N	4:D:27:SER:CB	2.59	0.60
5:T:123:VAL:HG23	5:T:233:ALA:HB3	1.84	0.60
5:T:169:ASP:HB2	5:T:186:LEU:HD12	1.82	0.60
5:J:147:PHE:CD2	5:J:148:PRO:CD	2.84	0.60
4:N:7:PRO:O	4:N:102:THR:HG23	2.01	0.60
4:D:158:LEU:HD22	4:D:167:SER:OG	2.01	0.60
5:E:19:MET:HG2	5:E:20:THR:N	2.15	0.60
4:N:190:ILE:HD13	4:N:190:ILE:H	1.66	0.59
2:Q:38:VAL:HG11	2:Q:61:TRP:CZ3	2.37	0.59
4:S:190:ILE:HD13	4:S:190:ILE:H	1.68	0.59
2:B:104:SER:HB3	2:B:114:LEU:HB3	1.84	0.59
4:D:65:THR:HG22	4:D:66:GLU:HG3	1.85	0.59
1:F:55:GLU:HG3	1:F:57:GLN:OE1	2.03	0.58
4:N:151:TYR:O	4:N:172:ALA:HA	2.03	0.58
4:D:158:LEU:HD23	4:D:158:LEU:O	2.03	0.58
2:L:4:ARG:O	2:L:6:ARG:NH1	2.35	0.58
4:N:169:SER:OG	5:O:189:ARG:HD3	2.03	0.58
5:O:147:PHE:CD2	5:O:148:PRO:CD	2.87	0.58
1:A:12:PHE:CE2	1:A:21:GLU:HG2	2.38	0.58
2:B:88:SER:HA	2:B:92:GLN:HG3	1.86	0.58
1:A:82:ILE:HD13	1:A:114:PRO:CD	2.16	0.58
1:A:90:THR:OG1	1:A:108:PHE:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:169:ASP:HB2	5:J:186:LEU:HD11	1.84	0.58
5:E:187:SER:OG	5:E:189:ARG:NH2	2.37	0.58
5:J:123:VAL:HG23	5:J:233:ALA:HB3	1.86	0.58
2:L:70:GLN:OE1	5:O:96:HIS:HD2	1.87	0.58
2:B:83:TYR:O	2:B:87:GLU:HB2	2.04	0.57
4:I:169:SER:HB2	5:J:189:ARG:HH11	1.68	0.57
2:B:126:SER:HA	6:B:197:HOH:O	2.04	0.57
2:G:49:ALA:O	4:N:161:ARG:NH1	2.37	0.57
2:Q:104:SER:O	2:Q:105:LYS:HD2	2.04	0.57
5:O:13:LEU:HD22	5:O:17:GLN:HB3	1.85	0.57
4:S:78:THR:HG21	4:S:166:LYS:HE2	1.86	0.57
2:B:67:LEU:HD13	5:E:96:HIS:CE1	2.39	0.57
5:E:94:THR:HG23	5:E:99:GLY:HA2	1.87	0.57
4:I:190:ILE:HD13	4:I:190:ILE:H	1.68	0.57
2:B:123:TYR:C	2:B:123:TYR:CD2	2.78	0.57
1:A:15:ASN:HB2	2:B:7:PHE:HB2	1.86	0.57
5:T:118:PRO:HD3	5:T:226:PRO:HB3	1.85	0.57
1:F:26:PHE:HB2	1:F:31:ILE:HD11	1.87	0.56
4:S:132:LEU:HD11	4:S:169:SER:HB2	1.86	0.56
1:A:160:VAL:HG13	1:A:177:HIS:CE1	2.40	0.56
3:C:37:ASP:OD2	3:C:37:ASP:N	2.27	0.56
5:E:36:ARG:HB3	5:E:46:ILE:HD11	1.88	0.56
2:L:97:PRO:HB3	2:L:122:PHE:HB3	1.87	0.56
4:S:47:TYR:CE2	4:S:49:PRO:HG3	2.41	0.56
1:K:129:THR:O	1:K:132:VAL:HG22	2.05	0.56
2:L:124:PRO:HD2	2:L:177:HIS:NE2	2.20	0.56
1:F:145:PHE:CZ	2:G:10:GLN:NE2	2.74	0.56
5:J:6:GLN:HE22	5:J:91:CYS:H	1.54	0.56
2:Q:81:HIS:O	2:Q:85:VAL:HG23	2.06	0.56
5:T:36:ARG:HB3	5:T:46:ILE:HD11	1.88	0.56
4:I:183:ASN:HA	4:I:186:ASN:HB3	1.88	0.56
2:B:119:VAL:HB	2:B:157:THR:HG22	1.88	0.56
1:F:76:ARG:HD2	2:G:53:LEU:CD2	2.36	0.56
1:K:162:ASP:OD1	1:K:177:HIS:HA	2.06	0.56
4:S:12:LEU:O	4:S:106:ILE:HA	2.06	0.56
4:I:158:LEU:HB3	5:J:167:CYS:HB2	1.88	0.55
4:S:6:SER:HB2	4:S:21:ARG:HB3	1.89	0.55
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.42	0.55
2:Q:124:PRO:CD	2:Q:177:HIS:CE1	2.90	0.55
2:B:39:ARG:O	2:B:39:ARG:HG3	2.05	0.55
4:I:24:PHE:O	4:I:67:ARG:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:116:ALA:O	4:N:133:PHE:HD1	1.89	0.55
5:O:148:PRO:HB3	5:O:150:HIS:ND1	2.21	0.55
5:O:94:THR:HG23	5:O:99:GLY:HA2	1.88	0.55
5:O:21:LEU:HD12	5:O:76:LEU:HD23	1.89	0.55
2:Q:73:ALA:CB	4:S:49:PRO:HB2	2.36	0.55
1:F:73:MET:SD	2:G:53:LEU:CD2	2.95	0.55
5:J:94:THR:HG23	5:J:99:GLY:CA	2.36	0.55
1:K:16:PRO:CD	1:K:17:ASP:H	2.17	0.55
2:L:18:PHE:HB2	2:L:23:ARG:HB3	1.89	0.55
5:O:15:ILE:HD12	5:O:111:GLU:HA	1.89	0.55
2:Q:87:GLU:HG3	2:Q:92:GLN:HE21	1.71	0.55
5:T:147:PHE:CD2	5:T:148:PRO:CD	2.90	0.55
4:I:36:GLN:HG2	4:I:37:ASN:H	1.71	0.55
1:P:82:ILE:HB	2:Q:33:ASN:ND2	2.22	0.54
2:Q:97:PRO:HB3	2:Q:122:PHE:HB3	1.90	0.54
2:B:86:GLY:HA2	2:B:89:PHE:CE2	2.42	0.54
4:S:158:LEU:HD11	5:T:191:ARG:HB2	1.89	0.54
4:S:78:THR:CG2	4:S:166:LYS:HE2	2.37	0.54
2:L:70:GLN:HE22	3:M:30:ASN:ND2	2.05	0.54
4:N:6:SER:CB	4:N:21:ARG:HB3	2.37	0.54
4:S:144:GLN:HA	4:S:144:GLN:HE21	1.72	0.54
2:G:83:TYR:O	2:G:87:GLU:HB2	2.07	0.54
5:T:10:PHE:CD1	5:T:150:HIS:HB3	2.42	0.54
2:B:152:ASP:O	2:B:153:TRP:HB2	2.07	0.54
1:K:3:GLU:HG2	1:K:4:GLU:H	1.72	0.54
4:N:181:CYS:HA	4:N:184:ALA:HB2	1.89	0.54
1:A:147:LYS:NZ	1:A:149:HIS:CE1	2.76	0.53
4:I:150:VAL:HA	4:I:174:SER:HB2	1.90	0.53
4:S:21:ARG:HG3	4:S:70:LEU:CD2	2.37	0.53
5:T:13:LEU:HD22	5:T:17:GLN:HB3	1.90	0.53
2:L:87:GLU:CG	2:L:92:GLN:NE2	2.71	0.53
1:A:168:TRP:NE1	2:B:3:THR:CG2	2.65	0.53
1:F:170:LEU:HD13	1:F:174:LEU:HB2	1.91	0.53
1:K:24:PHE:HB3	1:K:31:ILE:HD12	1.91	0.53
1:F:15:ASN:HB3	1:F:16:PRO:CD	2.38	0.53
2:L:144:SER:HB2	2:L:159:VAL:HG22	1.91	0.53
2:L:163:THR:HG22	2:L:164:VAL:N	2.24	0.53
2:G:156:GLN:O	2:G:156:GLN:NE2	2.37	0.53
2:L:85:VAL:HG11	3:M:26:ILE:HG13	1.90	0.53
4:N:67:ARG:CB	4:N:67:ARG:HH11	2.22	0.53
2:Q:8:LEU:H	2:Q:33:ASN:ND2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:ASN:HD22	4:I:141:ASN:ND2	2.07	0.52
4:I:31:LEU:HD22	4:I:69:SER:CB	2.39	0.52
1:P:113:THR:HB	1:P:144:LEU:HD23	1.91	0.52
2:L:4:ARG:HB2	2:L:5:PRO:HD2	1.90	0.52
4:N:67:ARG:NH1	4:N:67:ARG:HB2	2.24	0.52
4:D:158:LEU:C	4:D:158:LEU:CD2	2.78	0.52
2:Q:108:PRO:HB2	2:Q:111:HIS:CD2	2.45	0.52
1:A:109:ILE:CD1	1:A:119:VAL:HG21	2.39	0.52
5:E:37:GLN:HB2	5:E:43:LEU:HD23	1.92	0.52
2:G:67:LEU:HD13	5:J:96:HIS:CE1	2.44	0.52
1:A:28:GLY:O	1:A:146:ARG:NH2	2.43	0.52
2:L:132:PHE:HB2	2:L:172:THR:HB	1.92	0.52
5:E:34:TRP:NE1	5:E:76:LEU:HB2	2.24	0.52
2:Q:70:GLN:HE22	3:R:30:ASN:ND2	2.08	0.52
2:Q:87:GLU:CG	2:Q:92:GLN:HE21	2.22	0.52
5:T:14:LYS:HE3	5:T:112:ASP:HA	1.92	0.52
5:J:149:ASP:OD1	5:J:172:PRO:HG2	2.09	0.51
4:N:110:ILE:HD12	4:N:136:PHE:O	2.10	0.51
4:D:3:VAL:CG1	4:D:86:CYS:SG	2.98	0.51
5:J:30:ASN:ND2	5:J:50:VAL:O	2.43	0.51
5:J:6:GLN:HE21	5:J:102:GLY:HA3	1.75	0.51
2:L:55:ARG:N	2:L:56:PRO:HD2	2.25	0.51
2:L:70:GLN:OE1	5:O:96:HIS:CD2	2.64	0.51
4:N:160:MET:N	4:N:165:PHE:O	2.43	0.51
2:Q:107:GLN:O	2:Q:108:PRO:O	2.29	0.51
5:T:126:PRO:HD3	5:T:139:LEU:HG	1.93	0.51
5:E:126:PRO:HD3	5:E:139:LEU:HG	1.92	0.51
1:F:89:VAL:HG21	1:F:165:VAL:HG21	1.92	0.51
4:S:13:GLN:NE2	4:S:139:GLN:OE1	2.43	0.51
1:K:160:VAL:HG22	1:K:179:GLU:HB3	1.93	0.51
4:N:158:LEU:HB2	5:O:167:CYS:HB2	1.92	0.51
4:S:21:ARG:HG3	4:S:70:LEU:HD21	1.91	0.51
4:S:84:TYR:O	4:S:101:GLY:HA2	2.10	0.51
1:F:55:GLU:HB2	3:H:25:LEU:HD11	1.92	0.51
4:S:41:GLN:HE21	4:S:41:GLN:HA	1.76	0.51
1:A:105:LEU:HG	1:A:153:PHE:CE1	2.46	0.51
5:O:34:TRP:CE2	5:O:76:LEU:HB2	2.46	0.51
1:F:3:GLU:OE2	2:G:16:HIS:ND1	2.26	0.51
4:N:6:SER:HB3	4:N:7:PRO:CD	2.41	0.51
4:D:150:VAL:HA	4:D:174:SER:HB2	1.93	0.51
2:G:144:SER:C	2:G:146:GLY:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:87:ALA:HB2	4:N:98:PHE:CE2	2.46	0.50
2:B:19:ASN:ND2	2:B:22:GLU:OE1	2.41	0.50
1:K:16:PRO:HD2	1:K:17:ASP:N	2.25	0.50
4:S:181:CYS:HA	4:S:184:ALA:HB2	1.93	0.50
5:T:220:THR:HG22	5:T:221:GLN:NE2	2.24	0.50
3:H:36:ALA:O	3:H:37:ASP:C	2.50	0.50
4:S:5:GLN:HE21	4:S:99:GLY:HA3	1.76	0.50
4:I:5:GLN:HE22	4:I:85:PHE:HA	1.75	0.50
2:B:25:ARG:HD2	2:B:43:ASP:OD2	2.11	0.50
1:F:108:PHE:CE2	1:F:110:ASP:HB2	2.46	0.50
4:S:169:SER:OG	5:T:189:ARG:HD2	2.11	0.50
4:D:31:LEU:HD22	4:D:69:SER:HB2	1.94	0.50
2:Q:9:TRP:CH2	2:Q:30:CYS:HB3	2.47	0.50
5:T:92:ALA:HA	5:T:100:TYR:O	2.11	0.50
5:J:213:LEU:CD1	5:J:226:PRO:HG2	2.42	0.50
5:O:148:PRO:HB3	5:O:150:HIS:CE1	2.46	0.50
5:T:207:GLN:HA	5:T:232:SER:HB3	1.94	0.50
1:A:15:ASN:HB2	1:A:70:LEU:HD21	1.94	0.50
4:D:141:ASN:HD22	2:G:134:ASN:ND2	2.09	0.49
1:F:73:MET:SD	2:G:53:LEU:HD21	2.51	0.49
2:Q:132:PHE:CE2	2:Q:137:GLU:HG2	2.47	0.49
4:D:190:ILE:HD13	4:D:190:ILE:H	1.77	0.49
5:E:13:LEU:HD22	5:E:17:GLN:HB3	1.94	0.49
1:F:53:SER:HG	3:H:23:GLY:N	2.10	0.49
4:I:1:ILE:N	4:I:27:SER:HB2	2.27	0.49
5:E:33:TYR:CD1	5:E:33:TYR:N	2.81	0.49
4:I:36:GLN:CA	4:I:41:GLN:O	2.51	0.49
1:F:73:MET:SD	2:G:53:LEU:HD22	2.52	0.49
1:F:120:THR:OG1	1:F:164:ARG:HB3	2.12	0.49
5:O:198:GLN:HA	5:O:238:ARG:O	2.12	0.49
1:P:28:GLY:O	1:P:146:ARG:NH2	2.40	0.49
1:A:87:PRO:HB3	1:A:112:PHE:CD1	2.46	0.49
5:E:130:GLU:CD	5:E:138:THR:HG1	2.16	0.49
1:F:109:ILE:CD1	1:F:119:VAL:HG21	2.42	0.49
1:P:53:SER:OG	3:R:23:GLY:O	2.29	0.49
4:I:14:GLU:OE1	4:I:109:ASN:N	2.38	0.49
4:I:153:THR:HG21	5:J:187:SER:OG	2.13	0.49
2:Q:53:LEU:O	2:Q:56:PRO:HD2	2.12	0.49
1:K:55:GLU:HG2	4:N:93:ALA:HB2	1.95	0.49
4:N:5:GLN:HE21	4:N:101:GLY:HA2	1.78	0.49
5:J:94:THR:HG22	5:J:98:THR:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:9:GLN:HB3	2:Q:13:PHE:HB2	1.94	0.49
1:A:113:THR:HG23	1:A:114:PRO:HD2	1.93	0.48
4:S:145:SER:HB2	4:S:152:ILE:HD11	1.95	0.48
1:A:108:PHE:CE2	1:A:110:ASP:HB2	2.48	0.48
4:N:41:GLN:HE21	4:N:41:GLN:CA	2.24	0.48
5:J:6:GLN:NE2	5:J:91:CYS:H	2.10	0.48
5:O:92:ALA:HA	5:O:100:TYR:O	2.13	0.48
2:Q:36:GLU:HG2	2:Q:50:VAL:HG11	1.95	0.48
5:E:34:TRP:CE2	5:E:76:LEU:HB2	2.48	0.48
5:J:117:PHE:CD1	5:J:183:ARG:HD3	2.49	0.48
5:E:203:HIS:HB2	5:E:236:TRP:CZ3	2.48	0.48
2:Q:124:PRO:HD2	2:Q:124:PRO:O	2.13	0.48
4:D:36:GLN:HA	4:D:41:GLN:O	2.14	0.48
2:G:148:ILE:HB	2:G:156:GLN:NE2	2.28	0.48
1:K:94:ASN:HB3	1:K:103:ASN:OD1	2.13	0.48
4:N:6:SER:HB2	4:N:21:ARG:HB3	1.95	0.48
1:P:76:ARG:HD2	2:Q:53:LEU:CD2	2.42	0.48
2:Q:4:ARG:HB2	2:Q:5:PRO:HD2	1.95	0.48
2:B:174:GLN:HA	2:B:184:LEU:O	2.14	0.48
1:K:11:GLU:HG2	1:K:22:PHE:HD2	1.78	0.48
5:T:205:ARG:NH1	5:T:207:GLN:OE1	2.32	0.48
2:G:19:ASN:ND2	2:G:22:GLU:HG2	2.29	0.48
2:L:108:PRO:HB2	2:L:111:HIS:CD2	2.48	0.48
4:S:90:ILE:O	4:S:93:ALA:O	2.31	0.48
5:T:116:VAL:HG13	5:T:148:PRO:HG2	1.96	0.48
1:F:119:VAL:HG22	1:F:165:VAL:HG13	1.95	0.47
2:L:55:ARG:HG3	2:L:55:ARG:NH1	2.16	0.47
2:Q:18:PHE:HB2	2:Q:23:ARG:HB3	1.96	0.47
1:A:29:ASP:HB3	2:B:153:TRP:CE2	2.50	0.47
1:A:70:LEU:O	1:A:71:GLU:C	2.51	0.47
5:E:204:PHE:O	5:E:234:GLU:HA	2.14	0.47
1:F:9:GLN:O	1:F:9:GLN:HG2	2.13	0.47
4:N:12:LEU:O	4:N:106:ILE:HA	2.14	0.47
4:S:171:VAL:HG23	5:T:189:ARG:NH1	2.28	0.47
2:G:77:THR:HG22	4:I:29:ASN:OD1	2.13	0.47
3:M:24:GLU:OE1	4:N:26:ASP:HB2	2.13	0.47
4:I:35:HIS:O	4:I:83:VAL:O	2.32	0.47
5:O:11:ARG:HG2	5:O:19:MET:CE	2.44	0.47
4:S:41:GLN:HE21	4:S:41:GLN:CA	2.27	0.47
5:J:213:LEU:HD12	5:J:226:PRO:HG2	1.96	0.47
2:Q:75:VAL:HG13	2:Q:80:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:90:ILE:O	4:D:93:ALA:O	2.32	0.47
4:D:111:GLN:O	4:D:113:PRO:HD3	2.14	0.47
1:F:135:THR:HG23	1:F:148:PHE:HB2	1.97	0.47
1:K:15:ASN:HB2	1:K:70:LEU:HD21	1.95	0.47
4:N:67:ARG:CB	4:N:67:ARG:NH1	2.77	0.47
1:P:122:LEU:HB2	1:P:162:ASP:HB2	1.96	0.47
2:Q:81:HIS:HD2	2:Q:82:ASN:OD1	1.98	0.47
5:T:38:ASP:HB2	5:T:41:MET:HG3	1.96	0.47
5:T:225:LYS:HG2	5:T:227:VAL:HG13	1.96	0.47
5:E:77:ARG:HD3	5:E:79:GLU:OE2	2.14	0.47
2:G:123:TYR:C	2:G:123:TYR:CD2	2.87	0.47
4:N:74:SER:O	4:N:75:SER:C	2.52	0.47
4:S:41:GLN:HA	4:S:41:GLN:NE2	2.30	0.47
4:D:123:SER:HB3	5:E:125:GLU:OE2	2.15	0.47
1:K:16:PRO:CD	1:K:17:ASP:N	2.77	0.47
2:L:86:GLY:HA2	2:L:89:PHE:CZ	2.49	0.47
1:P:3:GLU:O	1:P:4:GLU:HB2	2.16	0.46
1:P:76:ARG:C	1:P:78:ASN:H	2.19	0.46
2:Q:8:LEU:H	2:Q:33:ASN:HD21	1.63	0.46
2:Q:88:SER:HA	2:Q:92:GLN:HG3	1.97	0.46
2:L:73:ALA:CB	4:N:49:PRO:HB2	2.45	0.46
4:S:24:PHE:CE1	4:S:67:ARG:HG2	2.50	0.46
1:A:15:ASN:HB3	1:A:16:PRO:HD3	1.98	0.46
5:J:90:PHE:HB3	5:J:101:PHE:HD2	1.80	0.46
2:L:124:PRO:HD3	2:L:177:HIS:CE1	2.50	0.46
5:T:45:LEU:HD11	5:T:48:TYR:HB3	1.96	0.46
2:B:163:THR:O	2:B:165:PRO:HD3	2.14	0.46
5:O:180:ASN:ND2	5:O:180:ASN:H	2.14	0.46
2:Q:130:ARG:NH1	2:Q:137:GLU:OE2	2.49	0.46
4:N:10:LEU:HD12	4:N:10:LEU:HA	1.76	0.46
4:N:182:ALA:HA	4:N:196:PHE:CE1	2.51	0.46
4:S:144:GLN:NE2	4:S:144:GLN:CA	2.77	0.46
4:D:143:SER:H	4:D:188:SER:HB3	1.80	0.46
4:D:163:MET:O	4:D:164:ASP:C	2.54	0.46
2:G:90:THR:OG1	2:G:91:VAL:N	2.49	0.46
4:N:6:SER:HB3	4:N:21:ARG:HB3	1.98	0.46
2:B:123:TYR:CD2	2:B:124:PRO:HA	2.51	0.46
4:N:21:ARG:HE	4:N:23:ASN:HD21	1.64	0.46
4:S:6:SER:HB3	4:S:7:PRO:HD2	1.98	0.46
2:G:74:ALA:O	2:G:78:TYR:HB3	2.16	0.46
5:O:12:ILE:HD11	5:O:212:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:144:GLN:HE21	4:S:144:GLN:CA	2.28	0.46
1:K:138:LEU:HB2	1:K:146:ARG:HB2	1.98	0.46
5:T:174:LYS:C	5:T:176:GLN:N	2.69	0.46
1:A:17:ASP:N	1:A:17:ASP:OD1	2.49	0.46
1:A:123:ARG:HD2	1:A:128:VAL:HG11	1.97	0.46
2:L:108:PRO:O	2:L:109:LEU:HB2	2.14	0.45
4:D:26:ASP:OD1	4:D:26:ASP:N	2.46	0.45
5:O:34:TRP:NE1	5:O:76:LEU:HB2	2.31	0.45
2:Q:108:PRO:O	2:Q:109:LEU:HB2	2.15	0.45
2:Q:110:GLN:HE21	2:Q:166:ARG:HG2	1.81	0.45
2:G:148:ILE:HB	2:G:156:GLN:HE21	1.80	0.45
4:I:196:PHE:HA	4:I:197:PRO:HD3	1.80	0.45
4:N:133:PHE:O	4:N:169:SER:HA	2.17	0.45
1:A:85:VAL:HA	1:A:86:PRO:HD3	1.82	0.45
4:I:90:ILE:O	4:I:93:ALA:O	2.35	0.45
4:I:94:GLN:HA	4:I:94:GLN:NE2	2.24	0.45
2:L:68:LEU:O	2:L:72:ARG:HG3	2.17	0.45
2:L:107:GLN:O	2:L:108:PRO:C	2.55	0.45
4:N:1:ILE:HG13	4:N:2:GLN:H	1.82	0.45
4:S:158:LEU:HD23	4:S:158:LEU:O	2.16	0.45
1:F:55:GLU:H	3:H:25:LEU:HD11	1.82	0.45
4:I:5:GLN:NE2	4:I:101:GLY:H	2.14	0.45
4:N:5:GLN:NE2	4:N:101:GLY:HA2	2.31	0.45
4:N:123:SER:HB3	5:O:125:GLU:OE2	2.15	0.45
5:J:13:LEU:HD11	5:J:19:MET:CB	2.47	0.45
1:K:108:PHE:CE2	1:K:110:ASP:HB2	2.52	0.45
4:D:122:ASP:HB2	4:D:128:LYS:HB2	1.98	0.45
1:F:135:THR:CG2	1:F:148:PHE:HB2	2.47	0.45
4:D:35:HIS:HE1	4:D:81:SER:O	1.99	0.45
4:I:110:ILE:HG13	4:I:137:ASP:HA	1.99	0.45
1:P:55:GLU:HG2	4:S:93:ALA:HB2	1.99	0.45
4:S:137:ASP:OD2	4:S:139:GLN:HB2	2.17	0.45
2:L:109:LEU:O	2:L:165:PRO:O	2.34	0.45
6:F:184:HOH:O	2:G:149:GLN:HG3	2.15	0.44
2:G:182:SER:HA	2:G:183:PRO:HD2	1.66	0.44
4:I:84:TYR:O	4:I:101:GLY:HA2	2.16	0.44
5:T:153:LEU:HD23	5:T:153:LEU:C	2.37	0.44
1:A:160:VAL:CG1	1:A:177:HIS:HE1	2.31	0.44
5:J:89:TYR:CD1	5:J:89:TYR:N	2.85	0.44
5:J:153:LEU:HG	5:J:208:VAL:HG22	1.99	0.44
2:L:70:GLN:HE22	3:M:30:ASN:HD21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:11:ARG:HG2	5:O:19:MET:HE3	1.99	0.44
4:S:37:ASN:ND2	4:S:41:GLN:HB3	2.32	0.44
1:F:113:THR:HG23	1:F:114:PRO:HD2	1.98	0.44
1:A:15:ASN:CB	2:B:7:PHE:HB2	2.47	0.44
3:M:37:ASP:OD2	3:M:37:ASP:N	2.45	0.44
5:J:203:HIS:HB2	5:J:236:TRP:CZ3	2.52	0.44
4:N:197:PRO:O	4:N:198:SER:C	2.55	0.44
4:S:152:ILE:HG23	4:S:172:ALA:HB2	1.98	0.44
4:S:171:VAL:HG12	4:S:173:TRP:HE3	1.83	0.44
1:A:15:ASN:CA	1:A:70:LEU:HD21	2.48	0.44
5:O:24:THR:HG23	5:O:73:ASP:OD1	2.17	0.44
4:S:107:ASN:HB3	4:S:138:SER:HB3	2.00	0.44
5:E:65:ASN:ND2	5:E:66:VAL:N	2.53	0.44
4:S:98:PHE:CZ	5:T:101:PHE:HZ	2.36	0.44
1:A:96:PRO:HG3	2:B:118:SER:OG	2.18	0.44
1:K:67:LYS:O	1:K:71:GLU:HG3	2.17	0.44
1:K:108:PHE:HD1	1:K:148:PHE:CE2	2.35	0.44
4:N:41:GLN:HA	4:N:41:GLN:NE2	2.31	0.44
4:N:52:THR:HA	4:N:60:ALA:O	2.18	0.44
5:T:14:LYS:O	5:T:17:GLN:HB2	2.18	0.44
4:I:51:GLY:O	4:I:61:THR:HA	2.18	0.44
1:K:141:GLU:OE2	2:L:29:ARG:NH2	2.51	0.44
2:L:166:ARG:O	2:L:167:SER:HB3	2.18	0.44
4:N:196:PHE:HA	4:N:197:PRO:HD3	1.88	0.44
2:B:46:GLU:OE2	2:B:48:ARG:NH1	2.51	0.43
2:G:67:LEU:O	2:G:71:ARG:HG2	2.18	0.43
5:J:28:ASN:HD22	5:J:28:ASN:HA	1.59	0.43
5:J:199:ASN:HB3	5:J:202:ASN:ND2	2.33	0.43
1:K:47:GLU:O	1:K:50:ARG:N	2.50	0.43
5:O:66:VAL:HG13	5:O:74:PHE:CE1	2.53	0.43
1:P:3:GLU:HG2	1:P:4:GLU:H	1.82	0.43
4:S:24:PHE:CD2	4:S:31:LEU:HD11	2.53	0.43
5:E:29:HIS:HB3	5:E:94:THR:O	2.18	0.43
4:I:24:PHE:CD2	4:I:31:LEU:HD13	2.53	0.43
1:K:47:GLU:O	1:K:48:PHE:C	2.55	0.43
2:Q:87:GLU:O	2:Q:92:GLN:HG3	2.18	0.43
4:S:54:GLN:HG2	4:S:55:ASN:N	2.33	0.43
2:B:119:VAL:HB	2:B:157:THR:CG2	2.48	0.43
5:E:94:THR:HG22	5:E:98:THR:C	2.38	0.43
2:G:129:VAL:HA	2:G:174:GLN:O	2.19	0.43
5:J:90:PHE:HB3	5:J:101:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:55:ARG:HH11	2:L:55:ARG:CG	2.22	0.43
3:M:24:GLU:HG3	3:M:25:LEU:H	1.83	0.43
5:O:94:THR:HG22	5:O:99:GLY:HA2	1.99	0.43
2:B:8:LEU:H	2:B:33:ASN:ND2	2.17	0.43
4:I:28:VAL:HG12	4:I:90:ILE:HA	1.99	0.43
1:P:108:PHE:CE2	1:P:110:ASP:HB2	2.54	0.43
2:Q:70:GLN:HE22	3:R:30:ASN:HD21	1.65	0.43
4:S:158:LEU:HB3	5:T:167:CYS:HB2	2.00	0.43
1:A:122:LEU:HD23	1:A:127:PRO:HA	2.01	0.43
1:P:22:PHE:HB3	1:P:34:VAL:HB	2.01	0.43
1:P:113:THR:O	1:P:167:HIS:CE1	2.71	0.43
1:P:113:THR:HG23	1:P:114:PRO:HD2	2.00	0.43
4:S:154:ASP:OD2	4:S:155:LYS:N	2.52	0.43
4:S:197:PRO:O	4:S:198:SER:C	2.57	0.43
5:T:117:PHE:CD1	5:T:183:ARG:HD3	2.54	0.43
1:A:7:ILE:HD12	2:B:17:PHE:CE1	2.53	0.43
2:L:93:ARG:HG2	2:L:123:TYR:CD2	2.53	0.43
2:L:124:PRO:CD	2:L:177:HIS:CE1	3.01	0.43
5:O:66:VAL:HG13	5:O:74:PHE:HE1	1.83	0.43
2:Q:4:ARG:O	2:Q:6:ARG:NH1	2.52	0.43
5:T:149:ASP:CG	5:T:149:ASP:O	2.57	0.43
1:A:147:LYS:HZ3	1:A:149:HIS:CE1	2.35	0.43
4:D:157:VAL:HG22	4:D:168:ASN:ND2	2.34	0.43
4:D:158:LEU:O	4:D:158:LEU:CD2	2.65	0.43
4:S:6:SER:CB	4:S:21:ARG:HB3	2.49	0.43
5:T:57:LYS:HB3	5:T:61:PRO:CG	2.48	0.43
5:J:141:CYS:HB2	5:J:155:TRP:CZ2	2.53	0.43
5:J:169:ASP:OD2	5:J:187:SER:OG	2.30	0.43
1:P:25:ASP:OD1	1:P:28:GLY:HA2	2.18	0.43
1:A:55:GLU:HG3	1:A:57:GLN:OE1	2.19	0.43
2:B:134:ASN:ND2	4:I:141:ASN:ND2	2.65	0.43
4:D:1:ILE:H3	4:D:27:SER:HB2	1.73	0.43
1:F:29:ASP:OD2	2:G:149:GLN:NE2	2.51	0.43
3:H:29:LEU:HD12	3:H:29:LEU:HA	1.95	0.43
4:N:160:MET:HB2	4:N:165:PHE:HB3	2.01	0.43
2:G:123:TYR:CD2	2:G:124:PRO:HA	2.54	0.42
1:K:70:LEU:HB2	2:L:9:TRP:HB2	2.00	0.42
5:T:19:MET:HG2	5:T:20:THR:N	2.34	0.42
5:T:120:GLU:O	5:T:143:ALA:HA	2.19	0.42
1:F:137:PHE:HB3	1:F:145:PHE:CD2	2.54	0.42
5:J:24:THR:HG22	5:J:25:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:ILE:CD1	1:K:119:VAL:HG21	2.48	0.42
2:L:87:GLU:HG3	2:L:92:GLN:NE2	2.34	0.42
4:N:26:ASP:OD1	4:N:67:ARG:NE	2.53	0.42
5:O:6:GLN:NE2	5:O:104:GLY:H	2.15	0.42
2:Q:124:PRO:CD	2:Q:124:PRO:O	2.67	0.42
2:B:19:ASN:HB3	2:B:22:GLU:HG2	2.01	0.42
1:F:9:GLN:NE2	1:F:11:GLU:OE2	2.47	0.42
5:J:147:PHE:CE2	5:J:148:PRO:HD3	2.54	0.42
4:N:13:GLN:HG2	4:N:109:ASN:OD1	2.20	0.42
4:N:26:ASP:OD1	4:N:67:ARG:NH2	2.52	0.42
4:S:51:GLY:O	4:S:61:THR:HA	2.20	0.42
4:S:52:THR:HA	4:S:60:ALA:O	2.19	0.42
2:B:68:LEU:HD23	2:B:68:LEU:HA	1.92	0.42
5:J:24:THR:HG22	5:J:25:GLN:H	1.83	0.42
4:N:67:ARG:HH11	4:N:67:ARG:HB3	1.83	0.42
2:Q:75:VAL:HG13	2:Q:80:ARG:NH1	2.35	0.42
1:F:172:GLU:HB2	1:F:173:PRO:HD2	2.02	0.42
1:K:39:LYS:HB3	1:K:60:LEU:HD21	2.02	0.42
4:S:87:ALA:HB2	4:S:98:PHE:CE2	2.54	0.42
1:A:160:VAL:HG13	1:A:177:HIS:HE1	1.81	0.42
4:D:3:VAL:HG13	4:D:86:CYS:SG	2.60	0.42
5:J:31:TYR:HA	5:J:49:SER:O	2.19	0.42
5:J:81:ALA:HA	5:J:85:GLN:OE1	2.19	0.42
2:Q:107:GLN:O	2:Q:108:PRO:C	2.58	0.42
2:G:144:SER:C	2:G:146:GLY:N	2.72	0.42
4:I:153:THR:HA	5:J:173:LEU:HD21	2.01	0.42
5:O:118:PRO:HD3	5:O:226:PRO:HB3	2.01	0.42
5:T:156:TRP:CE2	5:T:161:GLU:HG3	2.55	0.42
1:A:14:LEU:HD13	2:B:8:LEU:HD13	2.01	0.42
1:A:56:ALA:O	1:A:60:LEU:HD22	2.20	0.42
1:A:74:THR:HG23	2:B:7:PHE:CD2	2.55	0.42
2:B:187:GLU:OE1	2:B:189:ARG:NE	2.52	0.42
2:L:124:PRO:HD2	2:L:177:HIS:HE2	1.84	0.42
1:A:179:GLU:O	1:A:180:PHE:C	2.58	0.42
5:E:130:GLU:OE2	5:E:138:THR:OG1	2.37	0.42
1:F:160:VAL:HG11	1:F:177:HIS:NE2	2.35	0.42
1:P:109:ILE:CD1	1:P:119:VAL:HG21	2.49	0.42
5:E:31:TYR:HD1	5:E:50:VAL:HA	1.85	0.41
1:P:11:GLU:HG2	1:P:22:PHE:CD2	2.54	0.41
1:A:15:ASN:OD1	1:A:15:ASN:O	2.37	0.41
4:D:130:VAL:HG13	4:D:171:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:GLU:HG2	1:F:22:PHE:CD2	2.55	0.41
2:G:26:LEU:HD22	2:G:74:ALA:HB3	2.02	0.41
4:N:157:VAL:HG22	4:N:168:ASN:ND2	2.35	0.41
2:Q:18:PHE:CD1	2:Q:23:ARG:HG2	2.55	0.41
2:G:150:ASN:HB2	2:G:152:ASP:OD1	2.20	0.41
1:K:77:SER:O	1:K:80:THR:OG1	2.31	0.41
5:T:153:LEU:HD22	5:T:168:THR:OG1	2.20	0.41
4:D:76:SER:HB3	4:D:106:ILE:HG13	2.02	0.41
5:E:92:ALA:HA	5:E:100:TYR:O	2.20	0.41
2:G:99:VAL:HG21	2:G:175:VAL:HG21	2.02	0.41
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.86	0.41
2:Q:132:PHE:HB2	2:Q:172:THR:HB	2.02	0.41
4:D:107:ASN:HB3	4:D:138:SER:HB3	2.03	0.41
5:J:126:PRO:HG3	5:J:137:ALA:HB1	2.02	0.41
1:K:8:ILE:HB	1:K:25:ASP:HB3	2.03	0.41
4:I:60:ALA:HA	4:I:70:LEU:O	2.21	0.41
1:A:12:PHE:CD2	1:A:21:GLU:HG2	2.56	0.41
2:B:28:GLU:OE1	2:B:71:ARG:NE	2.48	0.41
4:I:133:PHE:HB2	4:I:185:PHE:CE2	2.56	0.41
1:K:9:GLN:HG3	1:K:24:PHE:CE1	2.56	0.41
2:L:163:THR:CG2	2:L:164:VAL:N	2.84	0.41
3:M:29:LEU:HD12	3:M:29:LEU:HA	2.00	0.41
4:N:48:ILE:HD13	4:N:53:LYS:HB2	2.02	0.41
5:O:130:GLU:OE2	5:O:138:THR:OG1	2.35	0.41
5:O:149:ASP:OD1	5:O:172:PRO:HG3	2.21	0.41
1:P:25:ASP:OD1	1:P:28:GLY:CA	2.69	0.41
1:P:118:ASN:HB3	1:P:166:GLU:HB2	2.03	0.41
2:Q:144:SER:HB2	2:Q:159:VAL:HG22	2.02	0.41
2:B:89:PHE:O	2:B:93:ARG:HB2	2.21	0.41
2:B:157:THR:C	2:B:158:LEU:HD12	2.41	0.41
4:D:145:SER:HA	4:D:187:ASN:OD1	2.20	0.41
1:K:38:LYS:O	1:K:40:GLU:HG2	2.21	0.41
5:O:14:LYS:O	5:O:17:GLN:HB2	2.21	0.41
1:P:3:GLU:OE2	2:Q:16:HIS:ND1	2.53	0.41
1:P:140:ARG:HD2	1:P:146:ARG:HG3	2.02	0.41
2:Q:86:GLY:HA2	2:Q:89:PHE:CZ	2.56	0.41
1:F:25:ASP:OD1	1:F:28:GLY:N	2.47	0.40
4:I:137:ASP:OD1	4:I:137:ASP:C	2.60	0.40
5:J:6:GLN:HA	5:J:22:GLN:O	2.21	0.40
4:N:6:SER:CB	4:N:7:PRO:CD	2.99	0.40
4:N:48:ILE:HG23	4:N:48:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:77:ARG:HG2	5:O:79:GLU:OE2	2.21	0.40
1:A:28:GLY:CA	1:A:146:ARG:HH22	2.34	0.40
1:A:119:VAL:HG11	1:A:149:HIS:CG	2.56	0.40
1:F:9:GLN:HB2	1:F:24:PHE:CZ	2.57	0.40
4:I:48:ILE:HD13	4:I:53:LYS:HB2	2.04	0.40
4:S:13:GLN:NE2	4:S:138:SER:HB2	2.36	0.40
4:S:57:ARG:NH2	4:S:80:ASP:OD1	2.38	0.40
4:S:133:PHE:O	4:S:169:SER:HA	2.20	0.40
5:T:181:ASP:OD2	5:T:181:ASP:N	2.41	0.40
2:B:134:ASN:HD22	4:I:141:ASN:HD22	1.67	0.40
1:F:85:VAL:HA	1:F:86:PRO:HD3	1.84	0.40
4:I:76:SER:HB3	4:I:106:ILE:HD12	2.02	0.40
4:I:136:PHE:HD1	4:I:140:THR:HB	1.87	0.40
5:J:49:SER:OG	5:J:68:ARG:NH1	2.50	0.40
1:K:113:THR:O	1:K:167:HIS:CE1	2.75	0.40
5:O:115:LYS:HA	5:O:115:LYS:HD2	1.86	0.40
5:T:156:TRP:CD1	5:T:156:TRP:N	2.89	0.40
1:A:15:ASN:CB	1:A:70:LEU:HD21	2.51	0.40
1:F:91:VAL:C	1:F:92:LEU:HD23	2.41	0.40
1:P:9:GLN:NE2	1:P:11:GLU:OE2	2.54	0.40
1:A:76:ARG:HH12	2:B:57:ASP:CG	2.25	0.40
2:G:122:PHE:CE1	2:G:156:GLN:HA	2.56	0.40
5:J:13:LEU:HD11	5:J:19:MET:HB2	2.03	0.40
4:N:31:LEU:HD23	4:N:69:SER:CB	2.46	0.40
1:P:76:ARG:HD2	2:Q:53:LEU:HD23	2.04	0.40
1:P:82:ILE:HD12	2:Q:33:ASN:HA	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:NZ	1:K:120:THR:CG2[1_656]	1.76	0.44

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	176/182 (97%)	162 (92%)	9 (5%)	5 (3%)	5	17
1	F	177/182 (97%)	165 (93%)	9 (5%)	3 (2%)	9	29
1	K	177/182 (97%)	165 (93%)	10 (6%)	2 (1%)	14	41
1	P	177/182 (97%)	160 (90%)	14 (8%)	3 (2%)	9	29
2	B	177/190 (93%)	161 (91%)	13 (7%)	3 (2%)	9	29
2	G	178/190 (94%)	161 (90%)	13 (7%)	4 (2%)	6	22
2	L	186/190 (98%)	172 (92%)	10 (5%)	4 (2%)	6	22
2	Q	186/190 (98%)	169 (91%)	13 (7%)	4 (2%)	6	22
3	C	13/15 (87%)	13 (100%)	0	0	100	100
3	H	13/15 (87%)	13 (100%)	0	0	100	100
3	M	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
3	R	13/15 (87%)	13 (100%)	0	0	100	100
4	D	196/202 (97%)	178 (91%)	15 (8%)	3 (2%)	10	33
4	I	196/202 (97%)	175 (89%)	16 (8%)	5 (3%)	5	18
4	N	196/202 (97%)	177 (90%)	15 (8%)	4 (2%)	7	24
4	S	196/202 (97%)	176 (90%)	14 (7%)	6 (3%)	4	14
5	E	236/240 (98%)	221 (94%)	13 (6%)	2 (1%)	19	49
5	J	237/240 (99%)	217 (92%)	16 (7%)	4 (2%)	9	29
5	O	236/240 (98%)	218 (92%)	14 (6%)	4 (2%)	9	29
5	T	236/240 (98%)	219 (93%)	14 (6%)	3 (1%)	12	36
All	All	3215/3316 (97%)	2947 (92%)	209 (6%)	59 (2%)	8	28

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
4	D	7	PRO
5	E	8	PRO
5	E	148	PRO
1	F	16	PRO
1	F	114	PRO
2	G	113	ASN
5	J	8	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	J	148	PRO
1	K	16	PRO
1	K	114	PRO
2	L	87	GLU
2	L	108	PRO
4	N	7	PRO
5	O	8	PRO
5	O	148	PRO
1	P	16	PRO
1	P	114	PRO
2	Q	108	PRO
2	Q	124	PRO
4	S	7	PRO
5	T	8	PRO
5	T	148	PRO
2	B	113	ASN
2	B	169	GLU
2	G	169	GLU
2	L	109	LEU
4	N	125	SER
1	P	4	GLU
2	Q	109	LEU
4	S	67	ARG
4	S	125	SER
5	T	135	GLN
1	A	27	ASP
4	D	125	SER
2	G	145	THR
5	J	180	ASN
2	L	124	PRO
4	N	128	LYS
4	N	197	PRO
5	O	63	GLY
4	S	128	LYS
4	S	197	PRO
4	I	7	PRO
4	I	36	GLN
2	Q	19	ASN
4	S	126	SER
4	D	164	ASP
1	F	136	VAL
2	G	124	PRO

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Mol	Chain	Res	Type
4	I	125	SER
5	J	15	ILE
4	I	80	ASP
5	O	39	PRO
4	I	3	VAL
1	A	136	VAL
2	B	124	PRO
1	A	16	PRO
1	A	96	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	163/166 (98%)	151 (93%)	12 (7%)	13	37
1	F	164/166 (99%)	157 (96%)	7 (4%)	29	62
1	K	164/166 (99%)	155 (94%)	9 (6%)	21	52
1	P	164/166 (99%)	152 (93%)	12 (7%)	14	38
2	B	163/171 (95%)	151 (93%)	12 (7%)	13	37
2	G	164/171 (96%)	152 (93%)	12 (7%)	14	38
2	L	170/171 (99%)	159 (94%)	11 (6%)	17	44
2	Q	170/171 (99%)	154 (91%)	16 (9%)	8	26
3	C	10/10 (100%)	7 (70%)	3 (30%)	0	1
3	H	10/10 (100%)	6 (60%)	4 (40%)	0	0
3	M	10/10 (100%)	7 (70%)	3 (30%)	0	1
3	R	10/10 (100%)	7 (70%)	3 (30%)	0	1
4	D	178/182 (98%)	155 (87%)	23 (13%)	4	13
4	I	178/182 (98%)	157 (88%)	21 (12%)	5	16
4	N	178/182 (98%)	161 (90%)	17 (10%)	8	24
4	S	178/182 (98%)	158 (89%)	20 (11%)	6	18
5	E	206/207 (100%)	191 (93%)	15 (7%)	14	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	J	206/207 (100%)	183 (89%)	23 (11%)	6	18
5	O	206/207 (100%)	183 (89%)	23 (11%)	6	18
5	T	206/207 (100%)	184 (89%)	22 (11%)	6	20
All	All	2898/2944 (98%)	2630 (91%)	268 (9%)	9	27

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	21	GLU
1	A	25	ASP
1	A	60	LEU
1	A	71	GLU
1	A	93	THR
1	A	97	VAL
1	A	129	THR
1	A	138	LEU
1	A	157	THR
1	A	175	LEU
1	A	176	LYS
2	B	3	THR
2	B	22	GLU
2	B	29	ARG
2	B	42	SER
2	B	53	LEU
2	B	92	GLN
2	B	113	ASN
2	B	120	SER
2	B	128	GLU
2	B	160	MET
2	B	166	ARG
2	B	180	VAL
3	C	25	LEU
3	C	30	ASN
3	C	37	ASP
4	D	13	GLN
4	D	18	SER
4	D	22	CYS
4	D	26	ASP
4	D	29	ASN
4	D	41	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	43	ILE
4	D	86	CYS
4	D	89	LEU
4	D	94	GLN
4	D	95	LYS
4	D	97	VAL
4	D	123	SER
4	D	125	SER
4	D	129	SER
4	D	130	VAL
4	D	156	CYS
4	D	158	LEU
4	D	178	ASP
4	D	183	ASN
4	D	188	SER
4	D	189	ILE
4	D	190	ILE
5	E	5	THR
5	E	17	GLN
5	E	25	GLN
5	E	33	TYR
5	E	47	TYR
5	E	59	GLU
5	E	65	ASN
5	E	66	VAL
5	E	79	GLU
5	E	87	SER
5	E	112	ASP
5	E	127	SER
5	E	180	ASN
5	E	189	ARG
5	E	214	SER
1	F	3	GLU
1	F	16	PRO
1	F	71	GLU
1	F	92	LEU
1	F	157	THR
1	F	158	GLU
1	F	171	ASP
2	G	22	GLU
2	G	29	ARG
2	G	35	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	G	53	LEU
2	G	75	VAL
2	G	113	ASN
2	G	120	SER
2	G	156	GLN
2	G	158	LEU
2	G	166	ARG
2	G	181	THR
2	G	182	SER
3	H	24	GLU
3	H	25	LEU
3	H	30	ASN
3	H	37	ASP
4	I	18	SER
4	I	21	ARG
4	I	31	LEU
4	I	41	GLN
4	I	74	SER
4	I	94	GLN
4	I	95	LYS
4	I	109	ASN
4	I	112	ASN
4	I	125	SER
4	I	129	SER
4	I	134	THR
4	I	144	GLN
4	I	151	TYR
4	I	156	CYS
4	I	158	LEU
4	I	169	SER
4	I	175	ASN
4	I	178	ASP
4	I	186	ASN
4	I	190	ILE
5	J	9	LYS
5	J	11	ARG
5	J	17	GLN
5	J	20	THR
5	J	25	GLN
5	J	28	ASN
5	J	66	VAL
5	J	69	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	J	77	ARG
5	J	87	SER
5	J	94	THR
5	J	107	LEU
5	J	112	ASP
5	J	128	GLU
5	J	144	THR
5	J	173	LEU
5	J	180	ASN
5	J	181	ASP
5	J	189	ARG
5	J	205	ARG
5	J	209	GLN
5	J	217	ASP
5	J	240	ASP
1	K	17	ASP
1	K	53	SER
1	K	60	LEU
1	K	93	THR
1	K	97	VAL
1	K	157	THR
1	K	160	VAL
1	K	171	ASP
1	K	181	ASP
2	L	4	ARG
2	L	53	LEU
2	L	55	ARG
2	L	75	VAL
2	L	98	LYS
2	L	128	GLU
2	L	156	GLN
2	L	160	MET
2	L	161	LEU
2	L	166	ARG
2	L	182	SER
3	M	25	LEU
3	M	30	ASN
3	M	37	ASP
4	N	6	SER
4	N	18	SER
4	N	29	ASN
4	N	41	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	N	74	SER
4	N	89	LEU
4	N	97	VAL
4	N	125	SER
4	N	141	ASN
4	N	148	SER
4	N	153	THR
4	N	156	CYS
4	N	158	LEU
4	N	164	ASP
4	N	179	PHE
4	N	190	ILE
4	N	192	GLU
5	O	17	GLN
5	O	19	MET
5	O	25	GLN
5	O	28	ASN
5	O	47	TYR
5	O	60	VAL
5	O	87	SER
5	O	112	ASP
5	O	115	LYS
5	O	128	GLU
5	O	132	SER
5	O	139	LEU
5	O	148	PRO
5	O	151	VAL
5	O	162	VAL
5	O	189	ARG
5	O	195	THR
5	O	201	ARG
5	O	209	GLN
5	O	220	THR
5	O	230	ILE
5	O	232	SER
5	O	240	ASP
1	P	40	GLU
1	P	55	GLU
1	P	60	LEU
1	P	88	GLU
1	P	92	LEU
1	P	97	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	P	133	SER
1	P	156	SER
1	P	157	THR
1	P	171	ASP
1	P	172	GLU
1	P	181	ASP
2	Q	4	ARG
2	Q	22	GLU
2	Q	34	GLN
2	Q	35	GLU
2	Q	48	ARG
2	Q	53	LEU
2	Q	75	VAL
2	Q	92	GLN
2	Q	109	LEU
2	Q	126	SER
2	Q	130	ARG
2	Q	136	GLN
2	Q	148	ILE
2	Q	166	ARG
2	Q	167	SER
2	Q	189	ARG
3	R	25	LEU
3	R	30	ASN
3	R	37	ASP
4	S	4	GLU
4	S	6	SER
4	S	26	ASP
4	S	29	ASN
4	S	41	GLN
4	S	78	THR
4	S	110	ILE
4	S	114	ASP
4	S	125	SER
4	S	141	ASN
4	S	144	GLN
4	S	149	ASP
4	S	152	ILE
4	S	156	CYS
4	S	158	LEU
4	S	164	ASP
4	S	179	PHE

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Mol	Chain	Res	Type
4	S	190	ILE
4	S	192	GLU
4	S	198	SER
5	T	17	GLN
5	T	18	SER
5	T	21	LEU
5	T	25	GLN
5	T	28	ASN
5	T	47	TYR
5	T	66	VAL
5	T	73	ASP
5	T	107	LEU
5	T	112	ASP
5	T	115	LYS
5	T	127	SER
5	T	128	GLU
5	T	132	SER
5	T	181	ASP
5	T	182	SER
5	T	189	ARG
5	T	195	THR
5	T	220	THR
5	T	227	VAL
5	T	232	SER
5	T	240	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	149	HIS
1	A	177	HIS
2	B	33	ASN
2	B	113	ASN
2	B	150	ASN
3	C	30	ASN
4	D	5	GLN
4	D	35	HIS
4	D	94	GLN
4	D	141	ASN
4	D	168	ASN
5	E	6	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	65	ASN
5	E	96	HIS
5	E	180	ASN
2	G	10	GLN
2	G	19	ASN
2	G	33	ASN
2	G	113	ASN
2	G	136	GLN
3	H	30	ASN
4	I	5	GLN
4	I	13	GLN
4	I	35	HIS
4	I	94	GLN
4	I	100	GLN
4	I	112	ASN
4	I	141	ASN
4	I	144	GLN
4	I	168	ASN
4	I	187	ASN
5	J	6	GLN
5	J	22	GLN
5	J	28	ASN
5	J	176	GLN
5	J	180	ASN
2	L	33	ASN
2	L	92	GLN
2	L	110	GLN
2	L	111	HIS
2	L	150	ASN
3	M	30	ASN
4	N	5	GLN
4	N	41	GLN
4	N	94	GLN
4	N	168	ASN
4	N	187	ASN
5	O	6	GLN
5	O	28	ASN
5	O	96	HIS
5	O	180	ASN
1	P	149	HIS
2	Q	33	ASN
2	Q	81	HIS

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Mol	Chain	Res	Type
2	Q	92	GLN
2	Q	110	GLN
2	Q	111	HIS
2	Q	113	ASN
2	Q	150	ASN
2	Q	156	GLN
3	R	30	ASN
4	S	5	GLN
4	S	13	GLN
4	S	41	GLN
4	S	77	GLN
4	S	144	GLN
4	S	168	ASN
5	T	6	GLN
5	T	22	GLN
5	T	28	ASN
5	T	96	HIS
5	T	221	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	178/182 (97%)	0.42	6 (3%) 45 35	6, 14, 20, 23	0
1	F	179/182 (98%)	0.53	9 (5%) 28 19	4, 15, 20, 30	0
1	K	179/182 (98%)	0.83	33 (18%) 1 1	10, 16, 22, 34	0
1	P	179/182 (98%)	0.70	19 (10%) 6 3	6, 16, 21, 28	0
2	B	181/190 (95%)	0.55	12 (6%) 18 11	3, 14, 18, 22	0
2	G	182/190 (95%)	0.50	8 (4%) 34 24	3, 13, 19, 28	0
2	L	188/190 (98%)	0.29	2 (1%) 80 75	4, 13, 19, 25	0
2	Q	188/190 (98%)	0.34	4 (2%) 63 54	4, 12, 18, 22	0
3	C	15/15 (100%)	0.22	0 100 100	2, 4, 15, 16	0
3	H	15/15 (100%)	0.43	1 (6%) 17 10	2, 7, 18, 19	0
3	M	15/15 (100%)	0.41	1 (6%) 17 10	3, 8, 21, 21	0
3	R	15/15 (100%)	0.23	0 100 100	4, 7, 17, 22	0
4	D	198/202 (98%)	0.56	13 (6%) 18 11	5, 15, 33, 35	0
4	I	198/202 (98%)	0.63	15 (7%) 13 7	4, 14, 41, 51	0
4	N	198/202 (98%)	0.62	22 (11%) 5 3	5, 14, 31, 35	0
4	S	198/202 (98%)	0.77	32 (16%) 1 1	5, 15, 31, 35	0
5	E	238/240 (99%)	0.20	1 (0%) 92 91	2, 12, 22, 24	0
5	J	239/240 (99%)	0.32	3 (1%) 77 72	3, 13, 24, 27	0
5	O	238/240 (99%)	0.21	4 (1%) 70 63	3, 13, 22, 27	0
5	T	238/240 (99%)	0.37	8 (3%) 45 35	5, 14, 21, 25	0
All	All	3259/3316 (98%)	0.47	193 (5%) 22 14	2, 14, 25, 51	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	177	SER	6.2
4	S	149	ASP	5.9
4	S	177	SER	5.9
4	N	192	GLU	4.9
4	N	193	ASP	4.7
4	N	191	PRO	4.5
4	D	186	ASN	4.4
1	F	129	THR	4.4
4	N	178	ASP	4.4
1	F	3	GLU	4.3
5	T	178	ALA	4.3
4	I	177	SER	4.3
2	G	167	SER	4.3
4	S	197	PRO	4.2
4	S	194	THR	4.1
4	S	198	SER	4.1
4	S	175	ASN	4.1
1	K	98	GLU	4.0
1	K	180	PHE	4.0
1	K	158	GLU	4.0
1	K	156	SER	4.0
2	G	113	ASN	4.0
4	I	178	ASP	3.9
1	P	129	THR	3.9
4	S	193	ASP	3.9
4	N	177	SER	3.9
4	N	1	ILE	3.8
1	P	177	HIS	3.8
1	P	158	GLU	3.8
5	T	179	LEU	3.8
4	N	198	SER	3.8
4	D	178	ASP	3.7
4	S	187	ASN	3.7
4	S	125	SER	3.7
1	A	100	ARG	3.7
4	D	176	LYS	3.6
4	N	197	PRO	3.6
1	P	171	ASP	3.6
1	P	126	LYS	3.6
4	S	185	PHE	3.6
4	N	126	SER	3.6
4	N	185	PHE	3.5
5	T	180	ASN	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	112	HIS	3.5
2	B	113	ASN	3.5
4	S	190	ILE	3.4
1	P	100	ARG	3.4
4	S	195	PHE	3.4
1	K	96	PRO	3.4
4	N	190	ILE	3.4
4	S	192	GLU	3.4
1	K	154	LEU	3.3
1	K	122	LEU	3.3
4	N	149	ASP	3.3
4	S	129	SER	3.2
1	F	177	HIS	3.2
4	S	191	PRO	3.2
4	S	186	ASN	3.2
1	K	100	ARG	3.2
4	S	150	VAL	3.2
1	K	159	ASP	3.2
1	K	179	GLU	3.2
4	N	175	ASN	3.1
5	T	18	SER	3.1
4	S	174	SER	3.1
2	Q	185	THR	3.1
4	I	194	THR	3.1
4	S	126	SER	3.1
1	P	160	VAL	3.1
2	L	18	PHE	3.1
4	N	196	PHE	3.1
4	S	178	ASP	3.1
4	D	198	SER	3.0
1	P	131	GLY	3.0
4	D	197	PRO	3.0
4	I	198	SER	3.0
1	K	155	PRO	3.0
5	T	61	PRO	3.0
4	D	183	ASN	3.0
1	K	153	PHE	3.0
2	B	88	SER	3.0
1	P	154	LEU	3.0
4	N	186	ASN	3.0
2	G	2	ASP	3.0
4	I	127	ASP	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	P	128	VAL	2.9
1	K	103	ASN	2.9
2	Q	189	ARG	2.9
1	P	130	THR	2.9
4	N	129	SER	2.9
4	N	4	GLU	2.9
4	I	190	ILE	2.8
1	K	123	ARG	2.8
4	I	191	PRO	2.8
2	B	161	LEU	2.8
5	O	218	GLU	2.8
4	N	187	ASN	2.8
1	K	3	GLU	2.8
5	O	220	THR	2.7
1	K	152	PRO	2.7
4	I	197	PRO	2.7
1	A	157	THR	2.7
4	D	192	GLU	2.7
5	E	180	ASN	2.7
2	B	165	PRO	2.7
2	L	185	THR	2.7
1	P	127	PRO	2.7
4	S	196	PHE	2.6
1	A	180	PHE	2.6
1	P	101	GLU	2.6
1	F	127	PRO	2.6
5	T	79	GLU	2.6
5	J	219	TRP	2.6
1	P	172	GLU	2.6
1	F	128	VAL	2.6
1	A	15	ASN	2.6
4	I	193	ASP	2.6
4	S	6	SER	2.6
4	I	186	ASN	2.6
4	S	144	GLN	2.5
1	K	131	GLY	2.5
3	H	23	GLY	2.5
1	P	122	LEU	2.5
2	B	173	CYS	2.5
1	P	170	LEU	2.5
2	G	186	VAL	2.5
1	K	171	ASP	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	K	172	GLU	2.5
2	B	143	VAL	2.5
1	P	157	THR	2.5
4	S	137	ASP	2.4
1	K	99	LEU	2.4
4	D	181	CYS	2.4
1	K	177	HIS	2.4
4	N	195	PHE	2.4
4	I	1	ILE	2.4
1	K	130	THR	2.4
4	S	1	ILE	2.4
5	O	134	THR	2.4
2	G	112	HIS	2.4
1	K	102	PRO	2.4
5	T	114	ASN	2.4
1	K	175	LEU	2.4
1	P	96	PRO	2.3
1	K	157	THR	2.3
4	I	192	GLU	2.3
1	A	99	LEU	2.3
5	T	134	THR	2.3
5	J	2	ALA	2.3
1	K	51	PHE	2.3
4	D	194	THR	2.3
1	A	158	GLU	2.3
4	I	109	ASN	2.3
4	I	183	ASN	2.3
1	K	127	PRO	2.3
2	B	144	SER	2.2
4	S	147	ASP	2.2
1	K	121	TRP	2.2
2	B	168	GLY	2.2
3	M	23	GLY	2.2
2	G	148	ILE	2.2
1	P	98	GLU	2.2
1	F	108	PHE	2.2
4	N	147	ASP	2.2
1	K	126	LYS	2.2
2	B	167	SER	2.2
4	S	148	SER	2.2
1	K	181	ASP	2.1
5	J	128	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
5	O	133	HIS	2.1
1	K	124	ASN	2.1
4	I	141	ASN	2.1
2	G	91	VAL	2.1
4	N	146	LYS	2.1
2	Q	176	GLU	2.1
4	S	183	ASN	2.1
1	K	97	VAL	2.1
4	S	123	SER	2.1
4	D	179	PHE	2.1
4	D	193	ASP	2.1
1	F	100	ARG	2.1
1	F	158	GLU	2.1
2	B	164	VAL	2.1
2	G	168	GLY	2.1
4	S	145	SER	2.1
2	Q	106	THR	2.1
4	D	126	SER	2.0
1	K	169	GLY	2.0
4	N	188	SER	2.0
1	F	157	THR	2.0
4	S	124	LYS	2.0
2	B	92	GLN	2.0
4	S	188	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.