



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:02 AM UTC

PDB ID : 2IAN / pdb_00002ian
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

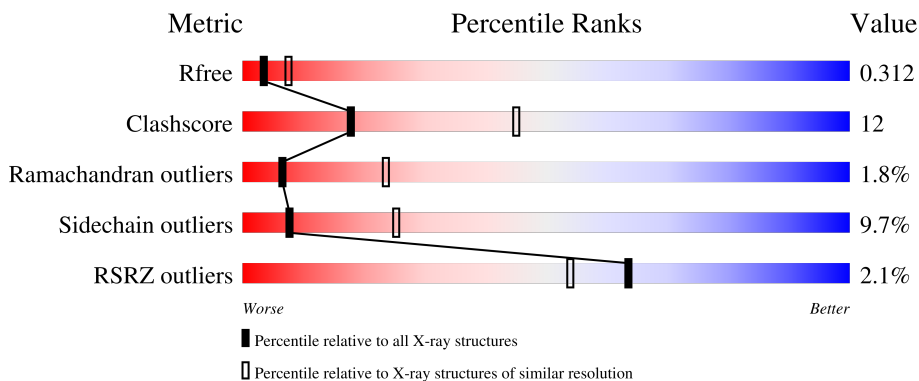
1 Overall quality at a glance i

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 ≥ 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	 2% 64% 26% 7% ..
1	F	182	 2% 69% 24% ..
1	K	182	 2% 68% 25% ..
1	P	182	 2% 70% 25% ...
2	B	190	 2% 63% 27% .. 5%

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Mol	Chain	Length	Quality of chain
2	G	190	<p>2% 66% 24% . . .</p>
2	L	190	<p>72% 23% . . .</p>
2	Q	190	<p>66% 27% 5% . .</p>
3	C	15	<p>67% 27% 7%</p>
3	H	15	<p>53% 27% 20%</p>
3	M	15	<p>60% 20% 20%</p>
3	R	15	<p>73% 20% 7%</p>
4	D	202	<p>3% 67% 24% 7% .</p>
4	I	202	<p>4% 61% 30% 7% .</p>
4	N	202	<p>7% 65% 28% . .</p>
4	S	202	<p>7% 61% 30% 7% .</p>
5	E	240	<p>78% 18% . .</p>
5	J	240	<p>66% 30% . .</p>
5	O	240	<p>71% 25% . . .</p>
5	T	240	<p>66% 28% . .</p>

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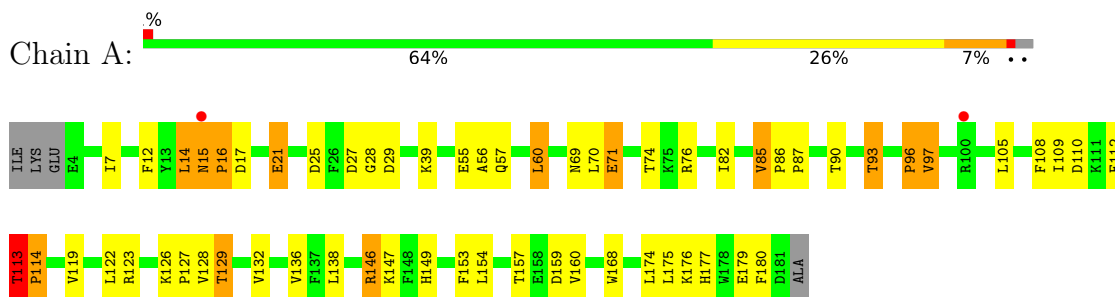
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	N	4	Total O 4 4	0	0
6	O	1	Total O 1 1	0	0
6	P	2	Total O 2 2	0	0
6	Q	2	Total O 2 2	0	0
6	S	2	Total O 2 2	0	0
6	T	6	Total O 6 6	0	0

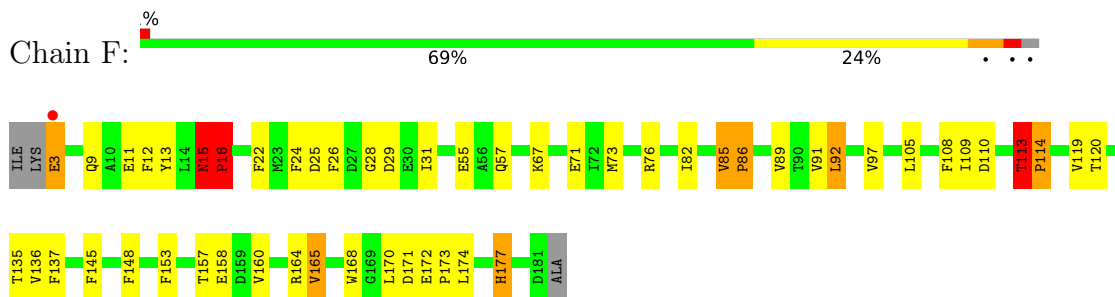
3 Residue-property plots [i](#)

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

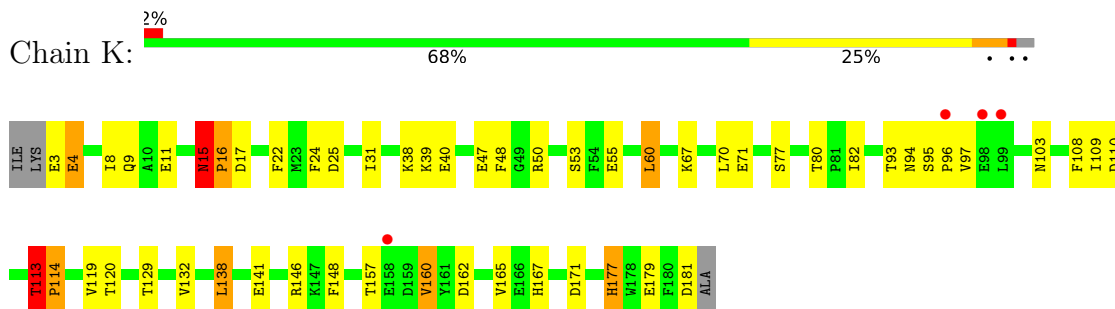
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



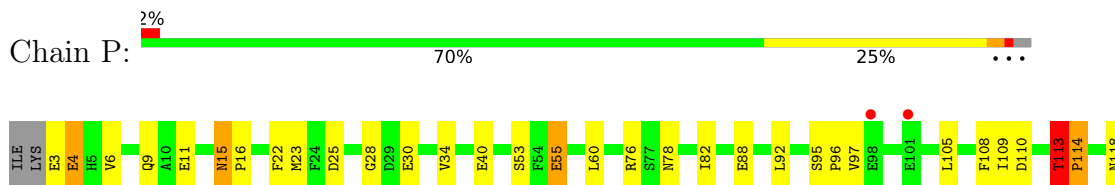
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



- 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



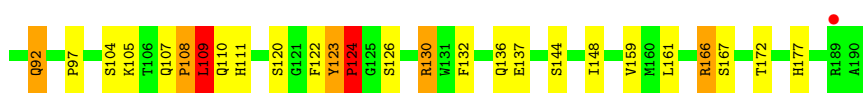
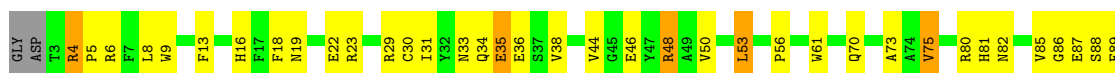
- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain



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



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

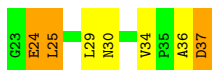


- Molecule 3: 15-mer peptide from Triosephosphate isomerase

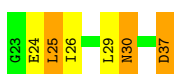




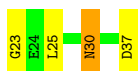
- Molecule 3: 15-mer peptide from Triosephosphate isomerase



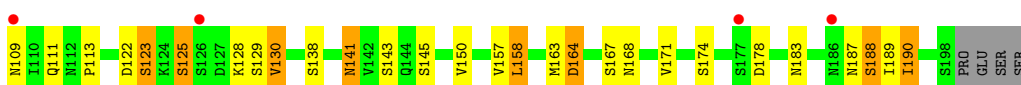
- Molecule 3: 15-mer peptide from Triosephosphate isomerase



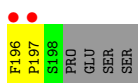
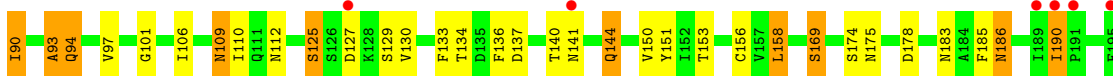
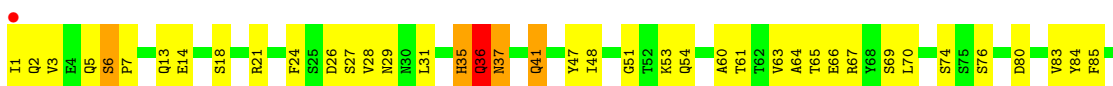
- Molecule 3: 15-mer peptide from Triosephosphate isomerase



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

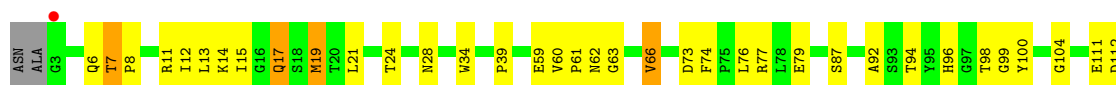


- Molecule 4: CD4+ T cell receptor E8 alpha chain

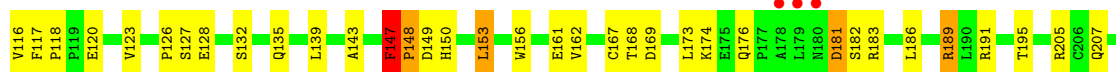




- Molecule 5: CD4+ T cell receptor E8 beta chain



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.296 0.252 , 0.312	Depositor DCC
R_{free} test set	5054 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtrriage
Anisotropy	0.509	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 11.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.71	0/1509	1.09	6/2058 (0.3%)
1	F	0.76	0/1518	1.13	7/2070 (0.3%)
1	K	0.61	0/1518	1.17	7/2070 (0.3%)
1	P	0.64	0/1518	1.08	4/2070 (0.2%)
2	B	0.79	0/1522	1.04	6/2066 (0.3%)
2	G	0.80	0/1530	1.09	9/2077 (0.4%)
2	L	0.70	1/1584 (0.1%)	0.98	4/2152 (0.2%)
2	Q	0.76	1/1584 (0.1%)	1.02	5/2152 (0.2%)
3	C	0.94	0/103	1.22	0/138
3	H	0.97	0/103	1.32	2/138 (1.4%)
3	M	0.84	0/103	1.06	0/138
3	R	0.79	0/103	0.96	0/138
4	D	0.82	1/1579 (0.1%)	1.09	6/2148 (0.3%)
4	I	0.83	2/1579 (0.1%)	1.14	10/2148 (0.5%)
4	N	0.77	0/1579	1.01	1/2148 (0.0%)
4	S	0.76	0/1579	1.03	4/2148 (0.2%)
5	E	0.79	0/1951	1.08	6/2659 (0.2%)
5	J	0.79	0/1956	1.12	10/2666 (0.4%)
5	O	0.72	0/1950	1.05	5/2658 (0.2%)
5	T	0.71	0/1951	0.96	6/2659 (0.2%)
All	All	0.75	5/26819 (0.0%)	1.07	98/36501 (0.3%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	35	HIS	C-O	-8.14	1.14	1.23
4	I	36	GLN	N-CA	6.94	1.55	1.46
4	D	35	HIS	C-O	-6.08	1.17	1.24
2	Q	166	ARG	C-O	-6.06	1.16	1.24
2	L	166	ARG	C-O	-5.62	1.16	1.24

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	147	PHE	CA-C-N	17.53	141.75	119.84
5	O	147	PHE	C-N-CA	17.53	141.75	119.84
1	K	15	ASN	CA-C-N	17.41	141.60	119.84
1	K	15	ASN	C-N-CA	17.41	141.60	119.84
1	F	113	THR	CA-C-N	15.67	136.52	120.38
1	F	113	THR	C-N-CA	15.67	136.52	120.38
1	A	113	THR	CA-C-N	15.03	135.86	120.38
1	A	113	THR	C-N-CA	15.03	135.86	120.38
1	K	113	THR	CA-C-N	14.44	135.26	120.38
1	K	113	THR	C-N-CA	14.44	135.26	120.38
2	Q	123	TYR	CA-C-N	14.23	137.63	119.84
2	Q	123	TYR	C-N-CA	14.23	137.63	119.84
5	J	7	THR	CA-C-N	14.19	137.58	119.84
5	J	7	THR	C-N-CA	14.19	137.58	119.84
4	D	6	SER	CA-C-N	13.73	134.52	120.38
4	D	6	SER	C-N-CA	13.73	134.52	120.38
1	P	15	ASN	CA-C-N	13.09	136.20	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	15	ASN	C-N-CA	13.09	136.20	119.84
1	P	113	THR	CA-C-N	12.76	133.52	120.38
1	P	113	THR	C-N-CA	12.76	133.52	120.38
5	E	147	PHE	CA-C-N	12.46	135.42	119.84
5	E	147	PHE	C-N-CA	12.46	135.42	119.84
4	I	6	SER	CA-C-N	11.24	131.96	120.38
4	I	6	SER	C-N-CA	11.24	131.96	120.38
5	J	147	PHE	CA-C-N	10.22	132.61	119.84
5	J	147	PHE	C-N-CA	10.22	132.61	119.84
2	G	123	TYR	CA-C-N	9.74	132.02	119.84
2	G	123	TYR	C-N-CA	9.74	132.02	119.84
5	E	7	THR	CA-C-N	9.57	131.81	119.84
5	E	7	THR	C-N-CA	9.57	131.81	119.84
2	L	123	TYR	CA-C-N	9.55	131.78	119.84
2	L	123	TYR	C-N-CA	9.55	131.78	119.84
2	B	123	TYR	CA-C-N	9.43	131.63	119.84
2	B	123	TYR	C-N-CA	9.43	131.63	119.84
2	L	166	ARG	N-CA-C	7.64	122.35	112.41
5	T	7	THR	CA-C-N	7.60	129.34	119.84
5	T	7	THR	C-N-CA	7.60	129.34	119.84
4	I	2	GLN	N-CA-C	7.36	121.77	110.36
5	O	7	THR	CA-C-N	7.24	128.90	119.84
5	O	7	THR	C-N-CA	7.24	128.90	119.84
2	G	182	SER	CA-C-N	7.03	128.63	119.84
2	G	182	SER	C-N-CA	7.03	128.63	119.84
1	A	15	ASN	O-C-N	6.93	126.65	120.48
2	G	3	THR	N-CA-C	6.86	120.82	108.48
4	S	161	ARG	N-CA-C	6.85	118.75	111.28
4	I	127	ASP	N-CA-C	6.80	118.77	111.36
4	S	127	ASP	N-CA-C	6.74	119.24	111.02
5	J	225	LYS	CA-C-N	6.70	128.21	119.84
5	J	225	LYS	C-N-CA	6.70	128.21	119.84
4	D	141	ASN	N-CA-C	6.63	119.54	108.20
1	F	15	ASN	CA-C-N	6.57	128.05	119.84
1	F	15	ASN	C-N-CA	6.57	128.05	119.84
5	J	3	GLY	N-CA-C	6.53	124.18	112.22
5	T	147	PHE	CA-C-N	6.46	127.92	119.84
5	T	147	PHE	C-N-CA	6.46	127.92	119.84
4	S	2	GLN	N-CA-C	6.39	119.18	110.55
4	D	2	GLN	N-CA-C	6.36	118.61	109.14
1	F	85	VAL	CA-C-N	6.14	124.08	119.66
1	F	85	VAL	C-N-CA	6.14	124.08	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	175	GLU	N-CA-C	-6.06	105.15	112.54
4	D	93	ALA	N-CA-C	-6.05	101.45	110.23
2	G	164	VAL	CA-C-N	6.01	125.97	119.78
2	G	164	VAL	C-N-CA	6.01	125.97	119.78
4	I	35	HIS	N-CA-C	5.95	120.61	112.04
1	A	85	VAL	CA-C-N	5.91	123.92	119.66
1	A	85	VAL	C-N-CA	5.91	123.92	119.66
2	G	124	PRO	N-CA-C	-5.82	100.49	112.47
5	J	94	THR	CB-CA-C	-5.71	99.06	110.42
4	I	35	HIS	O-C-N	-5.66	114.66	122.30
1	K	113	THR	CB-CA-C	5.64	118.08	109.56
1	A	159	ASP	N-CA-C	5.61	118.78	109.46
5	J	4	VAL	CB-CA-C	-5.57	103.58	111.21
2	L	124	PRO	N-CA-C	-5.50	101.13	112.47
4	N	152	ILE	N-CA-C	5.47	114.69	106.42
1	K	138	LEU	CA-C-N	5.45	125.92	120.14
1	K	138	LEU	C-N-CA	5.45	125.92	120.14
2	B	124	PRO	N-CA-C	-5.45	101.24	112.47
5	T	98	THR	N-CA-C	5.45	118.13	110.23
2	B	120	SER	N-CA-C	5.44	117.66	109.23
2	G	53	LEU	N-CA-C	-5.42	105.48	111.71
4	S	93	ALA	N-CA-C	-5.32	103.47	110.33
5	T	229	GLN	N-CA-C	5.26	115.47	108.38
2	Q	120	SER	N-CA-C	5.25	117.36	109.23
3	H	34	VAL	CA-C-N	-5.22	114.40	119.78
3	H	34	VAL	C-N-CA	-5.22	114.40	119.78
4	I	47	TYR	N-CA-C	-5.17	100.30	108.73
4	D	47	TYR	N-CA-C	-5.13	100.36	108.73
1	F	86	PRO	O-C-N	5.13	123.56	121.15
2	B	113	ASN	N-CA-C	5.12	121.70	110.80
2	B	17	PHE	N-CA-C	5.09	116.82	108.52
2	Q	44	VAL	N-CA-C	-5.09	107.78	111.90
2	Q	124	PRO	N-CA-C	-5.08	102.00	112.47
5	E	58	GLY	N-CA-C	-5.08	106.70	112.79
4	I	93	ALA	CA-C-N	-5.05	112.92	122.27
4	I	93	ALA	C-N-CA	-5.05	112.92	122.27
5	E	110	VAL	N-CA-C	5.05	115.85	108.53
5	J	120	GLU	N-CA-C	-5.03	102.33	110.32
4	I	37	ASN	N-CA-C	-5.01	98.73	109.81

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	49	1
1	F	1473	0	1407	42	0
1	K	1473	0	1407	33	1
1	P	1473	0	1407	31	0
2	B	1485	0	1416	45	0
2	G	1493	0	1420	43	0
2	L	1544	0	1478	41	0
2	Q	1544	0	1478	50	0
3	C	103	0	105	3	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	37	0
4	I	1546	0	1474	46	0
4	N	1546	0	1474	59	0
4	S	1546	0	1474	59	0
5	E	1896	0	1795	32	0
5	J	1901	0	1800	46	0
5	O	1895	0	1795	36	0
5	T	1896	0	1795	43	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	630	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 (630) 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
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
1:A:168:TRP:NE1	2:B:3:THR:HG21	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
5:O:11:ARG:HG2	5:O:19:MET:HE3	1.68	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:168:TRP:CD1	2:G:3:THR:HG1	2.05	0.74
4:D:158:LEU:C	4:D:158:LEU:HD23	2.13	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:86:THR:HG23	5:T:108:THR:HA	1.71	0.70
4:D:1:ILE:H1	4:D:27:SER:CB	2.04	0.70
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: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
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
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
2:B:90:THR:OG1	2:B:91:VAL:N	2.27	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
2:B:123:TYR:C	2:B:123:TYR:CD2	2.78	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:OG1	1:A:108:PHE:HB3	2.04	0.58
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:D:158:LEU:C	4:D:158:LEU:CD2	2.78	0.57
4:I:190:ILE:HD13	4:I:190:ILE:H	1.68	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:G:144:SER:C	2:G:146:GLY:H	2.13	0.55
2:Q:124:PRO:CD	2:Q:177:HIS:CE1	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:H:36:ALA:O	3:H:37:ASP:C	2.50	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
5:J:94:THR:HG22	5:J:98:THR:C	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:Q:108:PRO:HB2	2:Q:111:HIS:CD2	2.45	0.52
1:A:70:LEU:O	1:A:71:GLU:C	2.51	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
2:G:123:TYR:C	2:G:123:TYR:CD2	2.87	0.51
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
4:N:74:SER:O	4:N:75:SER:C	2.52	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
1:P:76:ARG:C	1:P:78:ASN:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:163:MET:O	4:D:164:ASP:C	2.54	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
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
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
2:L:107:GLN:O	2:L:108:PRO:C	2.55	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
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
5:T:153:LEU:HD23	5:T:153:LEU:C	2.37	0.49
1:A:87:PRO:HB3	1:A:112:PHE:CD1	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:N:197:PRO:O	4:N:198:SER:C	2.55	0.49
1:P:9:GLN:HB3	2:Q:13:PHE:HB2	1.94	0.49
5:T:174:LYS:C	5:T:176:GLN:N	2.69	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
1:K:47:GLU:O	1:K:48:PHE:C	2.55	0.48
5:E:94:THR:HG22	5:E:98:THR:C	2.38	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:F:168:TRP:NE1	2:G:3:THR:OG1	2.47	0.48
1:K:11:GLU:HG2	1:K:22:PHE:HD2	1.78	0.48
4:S:197:PRO:O	4:S:198:SER:C	2.57	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
5:T:149:ASP:CG	5:T:149:ASP:O	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:144:SER:C	2:G:146:GLY:N	2.72	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:23:MET:HE2	1:P:30:GLU:HG3	1.97	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
1:A:179:GLU:O	1:A:180:PHE:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:B:157:THR:C	2:B:158:LEU:HD12	2.41	0.45
2:G:148:ILE:HB	2:G:156:GLN:HE21	1.80	0.45
4:I:137:ASP:C	4:I:137:ASP:OD1	2.60	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
2:Q:107:GLN:O	2:Q:108:PRO:C	2.58	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
2:L:68:LEU:O	2:L:72:ARG:HG3	2.17	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
1:F:91:VAL:C	1:F:92:LEU:HD23	2.41	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
1:A:76:ARG:HH12	2:B:57:ASP:CG	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:P:130:THR:C	1:P:132:VAL:H	2.25	0.44
4:S:37:ASN:ND2	4:S:41:GLN:HB3	2.32	0.44
1:A:12:PHE:CD1	1:A:12:PHE:C	2.95	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: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
1:A:17:ASP:OD1	1:A:17:ASP:N	2.49	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
4:I:64:ALA:O	4:I:65:THR:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:D:1:ILE:H3	4:D:27:SER:HB2	1.72	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
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:31:ILE:HG23	2:Q:35:GLU:C	2.44	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
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
1:F:12:PHE:CD1	1:F:12:PHE:C	2.96	0.43
4:I:13:GLN:HE21	4:I:109:ASN:CG	2.27	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
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
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:31:ILE:HG23	2:B:35:GLU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:ASN:ND2	4:I:141:ASN:ND2	2.65	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:Q:166:ARG:O	2:Q:167:SER:C	2.61	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
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
1:F:168:TRP:CD1	2:G:3:THR:OG1	2.67	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
2:G:168:GLY:O	2:G:169:GLU:C	2.62	0.42
4:I:94:GLN:HA	4:I:94:GLN:NE2	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ALA:O	1:A:60:LEU:HD22	2.20	0.42
1:A:69:ASN:CG	3:C:34:VAL:HG13	2.45	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
5:J:51:GLY:O	5:J:52:ALA:C	2.63	0.42
2:L:124:PRO:HD2	2:L:177:HIS:HE2	1.84	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
5:J:214:SER:C	5:J:216:ASN:N	2.76	0.42
1:P:109:ILE:CD1	1:P:119:VAL:HG21	2.49	0.42
2:B:18:PHE:O	2:B:19:ASN:C	2.62	0.41
5:E:31:TYR:HD1	5:E:50:VAL:HA	1.85	0.41
4:N:19:THR:C	4:N:20:LEU:HD12	2.45	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
1:F:168:TRP:NE1	2:G:3:THR:HG1	2.18	0.41
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
2:L:163:THR:C	2:L:165:PRO:HD3	2.45	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
5:T:174:LYS:C	5:T:176:GLN:H	2.27	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
4:S:74:SER:O	4:S:75:SER:C	2.63	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
4:D:57:ARG:HH22	4:D:80:ASP:CG	2.28	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
5:J:180:ASN:C	5:J:180:ASN:HD22	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:S:127:ASP:O	4:S:128:LYS:C	2.63	0.41
2:B:89:PHE:O	2:B:93:ARG:HB2	2.21	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
1:K:95:SER:O	1:K:96:PRO:C	2.63	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
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
5:O:11:ARG:HG2	5:O:19:MET:CE	2.44	0.40
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
3:H:24:GLU:OE2	4:I:27:SER:OG	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:86:GLY:O	2:L:87:GLU:C	2.64	0.40
1:P:9:GLN:NE2	1:P:11:GLU:OE2	2.54	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%)	4	14
1	F	177/182 (97%)	165 (93%)	9 (5%)	3 (2%)	7	25
1	K	177/182 (97%)	165 (93%)	10 (6%)	2 (1%)	11	36
1	P	177/182 (97%)	160 (90%)	14 (8%)	3 (2%)	7	25
2	B	177/190 (93%)	161 (91%)	13 (7%)	3 (2%)	7	25
2	G	178/190 (94%)	161 (90%)	13 (7%)	4 (2%)	5	19
2	L	186/190 (98%)	172 (92%)	10 (5%)	4 (2%)	5	19
2	Q	186/190 (98%)	169 (91%)	13 (7%)	4 (2%)	5	19
3	C	13/15 (87%)	13 (100%)	0	0	100	100
3	H	13/15 (87%)	13 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	8	28
4	I	196/202 (97%)	175 (89%)	16 (8%)	5 (3%)	4	15
4	N	196/202 (97%)	177 (90%)	15 (8%)	4 (2%)	6	21
4	S	196/202 (97%)	176 (90%)	14 (7%)	6 (3%)	3	12
5	E	236/240 (98%)	221 (94%)	13 (6%)	2 (1%)	16	44
5	J	237/240 (99%)	217 (92%)	16 (7%)	4 (2%)	7	25
5	O	236/240 (98%)	218 (92%)	14 (6%)	4 (2%)	7	25
5	T	236/240 (98%)	219 (93%)	14 (6%)	3 (1%)	9	31
All	All	3215/3316 (97%)	2947 (92%)	209 (6%)	59 (2%)	6	23

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
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

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Mol	Chain	Res	Type
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
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%)	149 (91%)	14 (9%)	10	31
1	F	164/166 (99%)	154 (94%)	10 (6%)	17	46
1	K	164/166 (99%)	154 (94%)	10 (6%)	17	46
1	P	164/166 (99%)	150 (92%)	14 (8%)	10	31
2	B	163/171 (95%)	151 (93%)	12 (7%)	13	37
2	G	164/171 (96%)	149 (91%)	15 (9%)	9	28
2	L	170/171 (99%)	159 (94%)	11 (6%)	15	43
2	Q	170/171 (99%)	156 (92%)	14 (8%)	10	33
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%)	154 (86%)	24 (14%)	4	13
4	I	178/182 (98%)	155 (87%)	23 (13%)	4	14
4	N	178/182 (98%)	164 (92%)	14 (8%)	11	35
4	S	178/182 (98%)	159 (89%)	19 (11%)	6	21
5	E	206/207 (100%)	191 (93%)	15 (7%)	13	38
5	J	206/207 (100%)	182 (88%)	24 (12%)	5	18
5	O	206/207 (100%)	184 (89%)	22 (11%)	6	21
5	T	206/207 (100%)	180 (87%)	26 (13%)	4	15
All	All	2898/2944 (98%)	2618 (90%)	280 (10%)	8	25

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	25	ASP
1	A	39	LYS
1	A	60	LEU
1	A	71	GLU
1	A	93	THR
1	A	97	VAL
1	A	129	THR

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Mol	Chain	Res	Type
1	A	138	LEU
1	A	146	ARG
1	A	154	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	114	LEU
2	B	115	LEU
2	B	120	SER
2	B	128	GLU
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
4	D	43	ILE
4	D	58	LEU
4	D	86	CYS
4	D	89	LEU
4	D	90	ILE
4	D	94	GLN
4	D	97	VAL
4	D	109	ASN
4	D	123	SER
4	D	125	SER
4	D	129	SER
4	D	130	VAL
4	D	158	LEU
4	D	178	ASP
4	D	183	ASN

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Mol	Chain	Res	Type
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	59	GLU
5	E	65	ASN
5	E	66	VAL
5	E	79	GLU
5	E	87	SER
5	E	112	ASP
5	E	121	VAL
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	97	VAL
1	F	157	THR
1	F	158	GLU
1	F	165	VAL
1	F	171	ASP
1	F	177	HIS
2	G	22	GLU
2	G	29	ARG
2	G	35	GLU
2	G	53	LEU
2	G	75	VAL
2	G	113	ASN
2	G	114	LEU
2	G	115	LEU
2	G	120	SER
2	G	139	LYS
2	G	145	THR
2	G	156	GLN
2	G	158	LEU
2	G	181	THR

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Mol	Chain	Res	Type
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	41	GLN
4	I	54	GLN
4	I	74	SER
4	I	90	ILE
4	I	94	GLN
4	I	97	VAL
4	I	109	ASN
4	I	112	ASN
4	I	125	SER
4	I	129	SER
4	I	130	VAL
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
5	J	77	ARG
5	J	87	SER
5	J	94	THR
5	J	107	LEU
5	J	112	ASP
5	J	128	GLU

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Mol	Chain	Res	Type
5	J	144	THR
5	J	152	GLU
5	J	162	VAL
5	J	173	LEU
5	J	180	ASN
5	J	181	ASP
5	J	189	ARG
5	J	205	ARG
5	J	217	ASP
5	J	240	ASP
1	K	4	GLU
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	177	HIS
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	109	LEU
2	L	128	GLU
2	L	139	LYS
2	L	156	GLN
2	L	161	LEU
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	41	GLN
4	N	74	SER
4	N	77	GLN
4	N	89	LEU
4	N	97	VAL
4	N	109	ASN

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Mol	Chain	Res	Type
4	N	125	SER
4	N	148	SER
4	N	153	THR
4	N	158	LEU
4	N	190	ILE
4	N	192	GLU
5	O	17	GLN
5	O	19	MET
5	O	28	ASN
5	O	60	VAL
5	O	62	ASN
5	O	66	VAL
5	O	87	SER
5	O	112	ASP
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	179	LEU
5	O	189	ARG
5	O	195	THR
5	O	201	ARG
5	O	220	THR
5	O	230	ILE
5	O	232	SER
5	O	240	ASP
1	P	6	VAL
1	P	40	GLU
1	P	55	GLU
1	P	60	LEU
1	P	88	GLU
1	P	92	LEU
1	P	97	VAL
1	P	133	SER
1	P	156	SER
1	P	157	THR
1	P	171	ASP
1	P	172	GLU
1	P	175	LEU
1	P	181	ASP

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Mol	Chain	Res	Type
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	161	LEU
3	R	25	LEU
3	R	30	ASN
3	R	37	ASP
4	S	4	GLU
4	S	6	SER
4	S	13	GLN
4	S	41	GLN
4	S	43	ILE
4	S	73	ILE
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	158	LEU
4	S	163	MET
4	S	164	ASP
4	S	190	ILE
4	S	192	GLU
5	T	17	GLN
5	T	18	SER
5	T	25	GLN
5	T	28	ASN
5	T	44	LYS
5	T	66	VAL

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Mol	Chain	Res	Type
5	T	73	ASP
5	T	80	LEU
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	153	LEU
5	T	162	VAL
5	T	173	LEU
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	230	ILE
5	T	232	SER
5	T	240	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	15	ASN
1	A	149	HIS
1	A	177	HIS
2	B	10	GLN
2	B	33	ASN
2	B	113	ASN
2	B	156	GLN
3	C	30	ASN
4	D	5	GLN
4	D	35	HIS
4	D	94	GLN
4	D	141	ASN
4	D	168	ASN
4	D	186	ASN
5	E	6	GLN
5	E	22	GLN
5	E	65	ASN

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Mol	Chain	Res	Type
5	E	96	HIS
5	E	150	HIS
5	E	176	GLN
2	G	10	GLN
2	G	19	ASN
2	G	33	ASN
3	H	30	ASN
4	I	5	GLN
4	I	13	GLN
4	I	44	ASN
4	I	77	GLN
4	I	94	GLN
4	I	100	GLN
4	I	112	ASN
4	I	119	GLN
4	I	141	ASN
4	I	144	GLN
4	I	168	ASN
4	I	187	ASN
5	J	6	GLN
5	J	28	ASN
5	J	176	GLN
5	J	180	ASN
1	K	149	HIS
2	L	10	GLN
2	L	33	ASN
2	L	34	GLN
2	L	92	GLN
2	L	111	HIS
2	L	150	ASN
2	L	156	GLN
2	L	174	GLN
3	M	30	ASN
4	N	5	GLN
4	N	36	GLN
4	N	41	GLN
4	N	44	ASN
4	N	94	GLN
4	N	168	ASN
4	N	183	ASN
4	N	187	ASN
5	O	6	GLN

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Mol	Chain	Res	Type
5	O	22	GLN
5	O	28	ASN
5	O	37	GLN
5	O	65	ASN
5	O	96	HIS
5	O	135	GLN
5	O	180	ASN
5	O	209	GLN
1	P	84	ASN
1	P	149	HIS
2	Q	33	ASN
2	Q	81	HIS
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	109	ASN
4	S	144	GLN
4	S	168	ASN
4	S	183	ASN
5	T	6	GLN
5	T	22	GLN
5	T	28	ASN
5	T	96	HIS
5	T	135	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 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	178/182 (97%)	0.19	2 (1%) 78 70	6, 14, 20, 23	0
1	F	179/182 (98%)	0.22	1 (0%) 85 80	4, 15, 20, 30	0
1	K	179/182 (98%)	0.33	4 (2%) 62 52	10, 16, 22, 34	0
1	P	179/182 (98%)	0.32	3 (1%) 69 60	6, 16, 21, 28	0
2	B	181/190 (95%)	0.17	2 (1%) 78 70	3, 14, 18, 22	0
2	G	182/190 (95%)	0.20	3 (1%) 70 61	3, 13, 19, 28	0
2	L	188/190 (98%)	-0.01	0 100 100	4, 13, 19, 25	0
2	Q	188/190 (98%)	0.03	1 (0%) 87 82	4, 12, 18, 22	0
3	C	15/15 (100%)	0.01	0 100 100	2, 4, 15, 16	0
3	H	15/15 (100%)	0.19	0 100 100	2, 7, 18, 19	0
3	M	15/15 (100%)	0.04	0 100 100	3, 8, 21, 21	0
3	R	15/15 (100%)	-0.02	0 100 100	4, 7, 17, 22	0
4	D	198/202 (98%)	0.31	6 (3%) 52 42	5, 15, 33, 35	0
4	I	198/202 (98%)	0.40	9 (4%) 38 30	4, 14, 41, 51	0
4	N	198/202 (98%)	0.38	15 (7%) 20 14	5, 14, 31, 35	0
4	S	198/202 (98%)	0.41	14 (7%) 22 16	5, 15, 31, 35	0
5	E	238/240 (99%)	0.00	1 (0%) 88 84	2, 12, 22, 24	0
5	J	239/240 (99%)	0.10	2 (0%) 82 75	3, 13, 24, 27	0
5	O	238/240 (99%)	0.07	1 (0%) 88 84	3, 13, 22, 27	0
5	T	238/240 (99%)	0.17	3 (1%) 75 66	5, 14, 21, 25	0
All	All	3259/3316 (98%)	0.20	67 (2%) 63 54	2, 14, 25, 51	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	1	ILE	4.5
4	I	190	ILE	3.6
4	S	149	ASP	3.4
4	N	1	ILE	3.4
4	S	177	SER	3.3
1	K	98	GLU	3.3
4	I	141	ASN	3.2
1	F	3	GLU	3.2
4	N	178	ASP	3.1
4	S	187	ASN	3.0
4	N	192	GLU	3.0
4	N	126	SER	2.9
4	N	149	ASP	2.9
1	P	160	VAL	2.8
4	S	185	PHE	2.8
4	D	1	ILE	2.8
5	J	2	ALA	2.8
2	B	113	ASN	2.7
4	N	187	ASN	2.7
4	I	197	PRO	2.7
2	B	112	HIS	2.7
2	G	113	ASN	2.7
4	N	129	SER	2.7
4	S	197	PRO	2.6
4	D	186	ASN	2.6
4	S	1	ILE	2.6
1	A	100	ARG	2.6
1	K	99	LEU	2.5
5	T	180	ASN	2.5
4	N	193	ASP	2.5
1	K	96	PRO	2.4
5	E	231	VAL	2.4
2	Q	189	ARG	2.4
4	D	126	SER	2.4
4	S	189	ILE	2.4
4	S	125	SER	2.4
4	N	186	ASN	2.4
4	N	197	PRO	2.4
1	K	158	GLU	2.3
5	T	179	LEU	2.3
4	D	177	SER	2.3
2	G	2	ASP	2.2
4	N	131	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
4	I	191	PRO	2.2
1	P	98	GLU	2.2
5	T	178	ALA	2.2
1	A	15	ASN	2.2
1	P	101	GLU	2.2
4	S	186	ASN	2.2
4	S	144	GLN	2.2
4	D	39	TRP	2.2
4	I	196	PHE	2.2
2	G	167	SER	2.1
4	N	177	SER	2.1
4	N	198	SER	2.1
4	S	181	CYS	2.1
4	S	188	SER	2.1
4	I	195	PHE	2.1
4	N	147	ASP	2.1
5	J	215	GLU	2.1
4	S	174	SER	2.1
4	S	126	SER	2.0
4	N	185	PHE	2.0
4	I	189	ILE	2.0
4	D	109	ASN	2.0
5	O	3	GLY	2.0
4	I	127	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.