



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:32 am BST

PDB ID : 2FJF
Title : Structure of the G6 Fab, a phage derived VEGF binding Fab
Authors : Wiesmann, C.
Deposited on : 2006-01-02
Resolution : 2.65 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 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 : 2.11
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) : 2.11

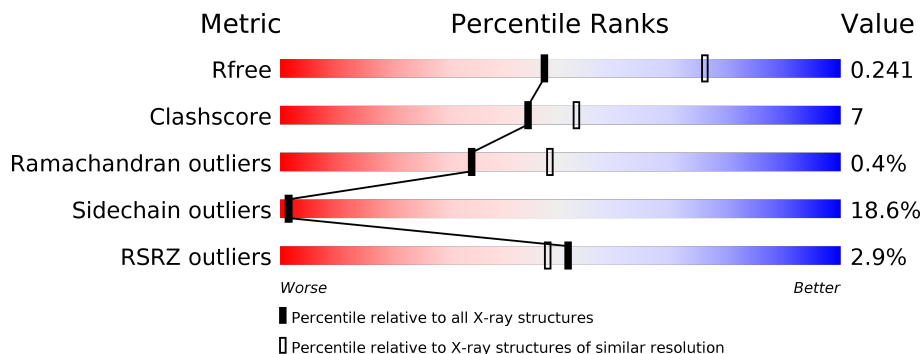
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	214	 2% 64% 28% 6%
1	C	214	 % 72% 23%
1	E	214	 73% 21%
1	G	214	 75% 18% 5%
1	J	214	 74% 22%
1	L	214	 3% 74% 20% 5%

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Mol	Chain	Length	Quality of chain
1	M	214	 12% 69% 23% 7%
1	O	214	 % 69% 25%
1	Q	214	 5% 69% 23% 6%
1	S	214	 4% 69% 24% 5%
1	U	214	 3% 65% 28% 5%
1	W	214	 2% 66% 30%
2	B	227	 3% 68% 26%
2	D	227	 3% 76% 18%
2	F	227	 4% 71% 22%
2	H	227	 5% 72% 21%
2	I	227	 % 67% 26%
2	K	227	 3% 71% 22%
2	N	227	 7% 71% 22%
2	P	227	 74% 19%
2	R	227	 4% 68% 24%
2	T	227	 2% 67% 24%
2	V	227	 2% 70% 22%
2	X	227	 2% 73% 20%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 39642 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 Light Chain of a VEGF binding Antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1617	1014	268	330	5	0	0	0
1	A	211	1617	1014	268	330	5	0	0	0
1	C	211	1617	1014	268	330	5	0	0	0
1	E	211	1617	1014	268	330	5	0	0	0
1	G	211	1617	1014	268	330	5	0	0	0
1	J	211	1617	1014	268	330	5	0	0	0
1	M	211	1617	1014	268	330	5	0	0	0
1	O	211	1617	1014	268	330	5	0	0	0
1	Q	211	1617	1014	268	330	5	0	0	0
1	S	211	1617	1014	268	330	5	0	0	0
1	U	211	1617	1014	268	330	5	0	0	0
1	W	211	1617	1014	268	330	5	0	0	0

- Molecule 2 is a protein called Heavy Chain of a VEGF binding Antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	218	1633	1044	267	315	7	0	0	0
2	B	218	1633	1044	267	315	7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	F	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	I	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	K	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	N	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	P	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	R	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	T	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	V	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	X	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	22	Total	O	0	0
			22	22		
3	H	44	Total	O	0	0
			44	44		
3	A	17	Total	O	0	0
			17	17		
3	B	28	Total	O	0	0
			28	28		
3	C	10	Total	O	0	0
			10	10		
3	D	30	Total	O	0	0
			30	30		
3	E	14	Total	O	0	0
			14	14		
3	F	30	Total	O	0	0
			30	30		
3	G	53	Total	O	0	0
			53	53		

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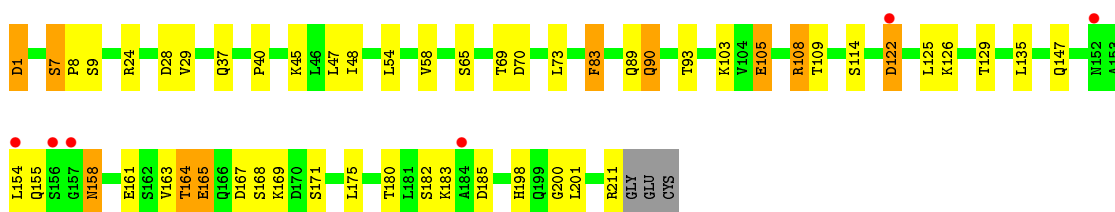
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	52	Total 52	O 52	0	0
3	J	35	Total 35	O 35	0	0
3	K	53	Total 53	O 53	0	0
3	M	17	Total 17	O 17	0	0
3	N	24	Total 24	O 24	0	0
3	O	31	Total 31	O 31	0	0
3	P	52	Total 52	O 52	0	0
3	Q	15	Total 15	O 15	0	0
3	R	21	Total 21	O 21	0	0
3	S	9	Total 9	O 9	0	0
3	T	15	Total 15	O 15	0	0
3	U	16	Total 16	O 16	0	0
3	V	28	Total 28	O 28	0	0
3	W	5	Total 5	O 5	0	0
3	X	21	Total 21	O 21	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

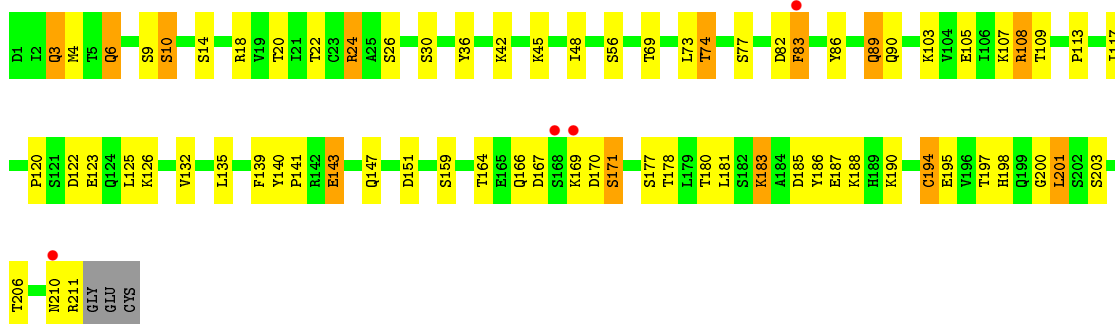
- Molecule 1: Light Chain of a VEGF binding Antibody

Chain L: 



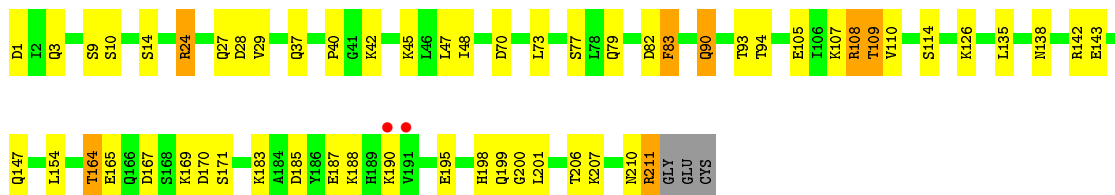
- Molecule 1: Light Chain of a VEGF binding Antibody

Chain A: 



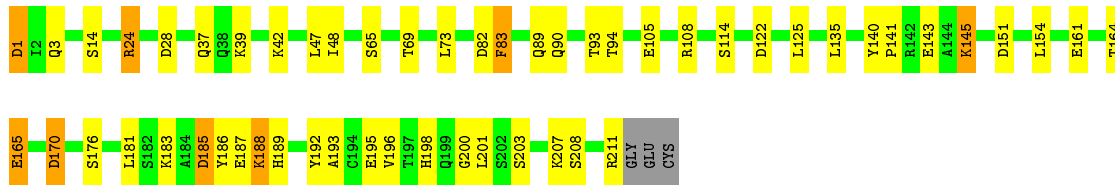
- Molecule 1: Light Chain of a VEGF binding Antibody

Chain C: 




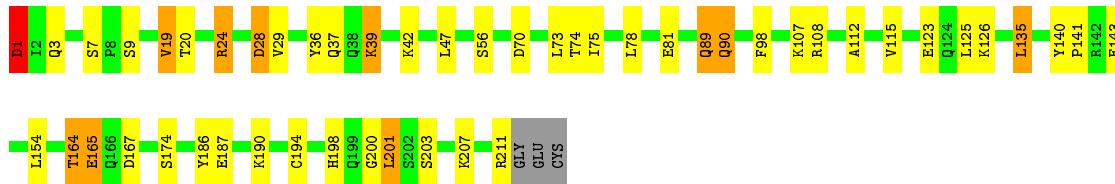
- Molecule 1: Light Chain of a VEGF binding Antibody

Chain E:  73% 21%



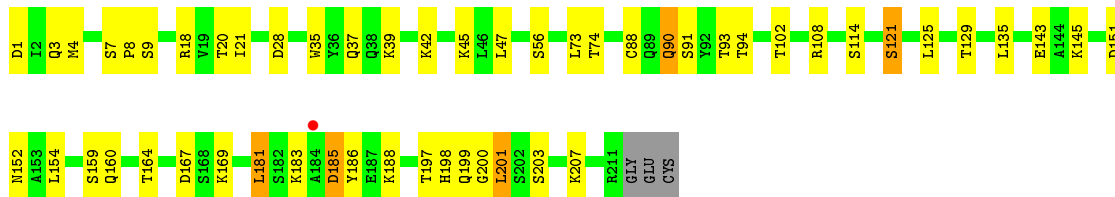
• Molecule 1: Light Chain of a VEGF binding Antibody

Chain G:  75% 18% 5%



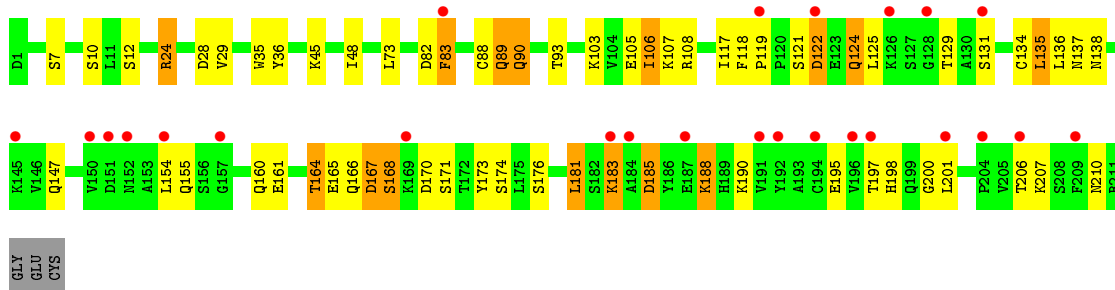
• Molecule 1: Light Chain of a VEGF binding Antibody

Chain J:  74% 22%



• Molecule 1: Light Chain of a VEGF binding Antibody

Chain M:  12% 69% 23% 7%



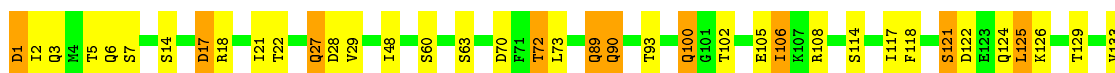
• Molecule 1: Light Chain of a VEGF binding Antibody

Chain O:  69% 25%

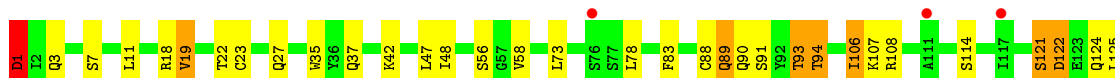




• Molecule 1: Light Chain of a VEGF binding Antibody



• Molecule 1: Light Chain of a VEGF binding Antibody



• Molecule 1: Light Chain of a VEGF binding Antibody



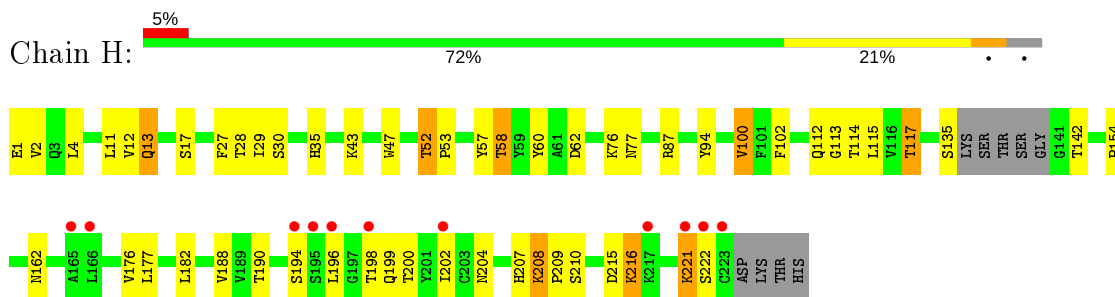
GLY
GLU
CYS

• Molecule 1: Light Chain of a VEGF binding Antibody

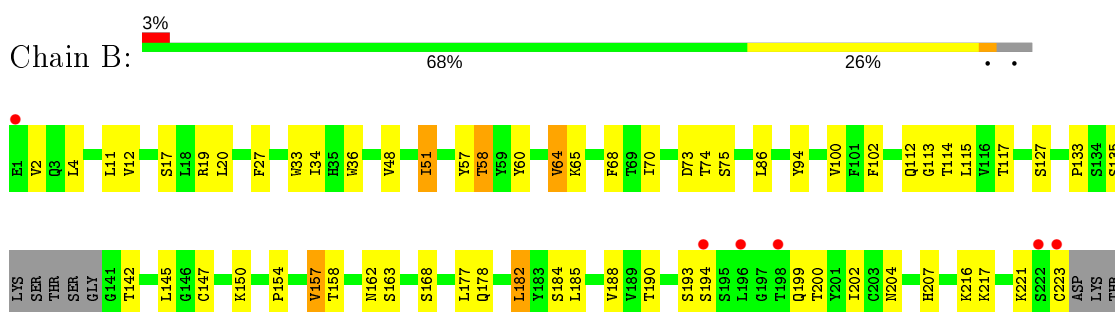


CYS

- Molecule 2: Heavy Chain of a VEGF binding Antibody

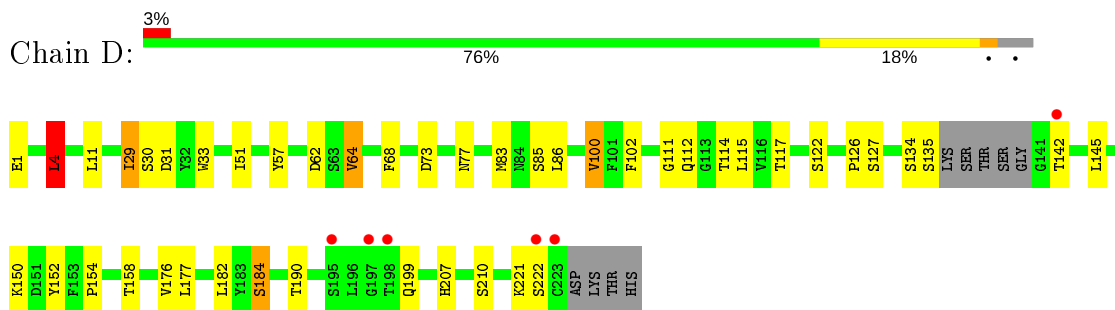


- Molecule 2: Heavy Chain of a VEGF binding Antibody

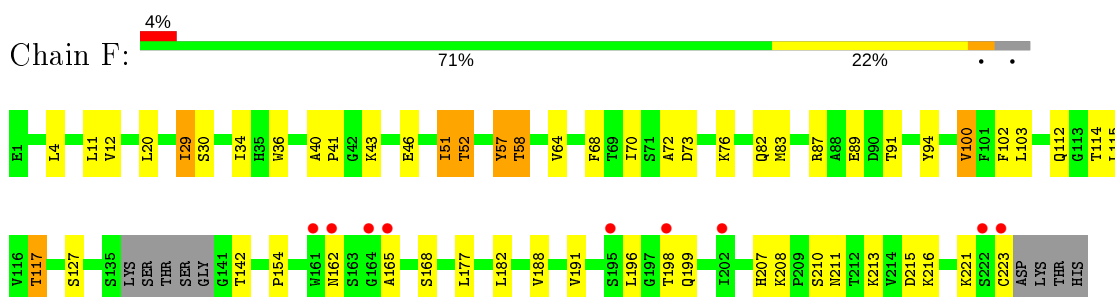


HIS

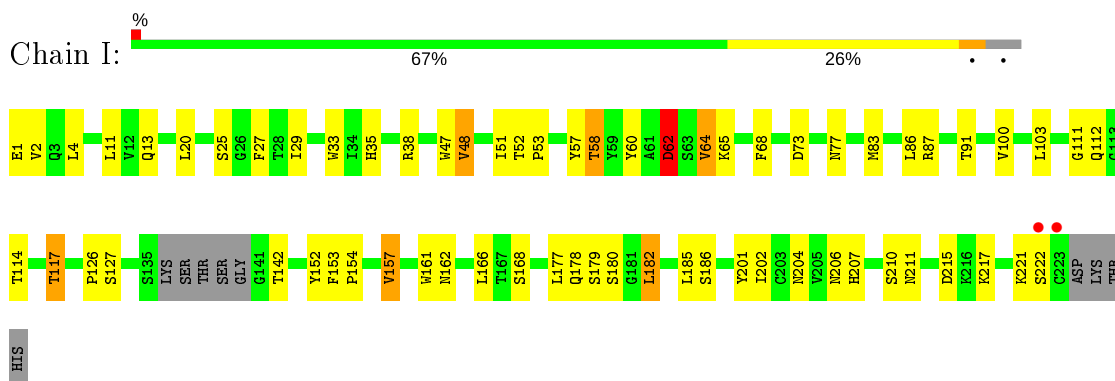
- Molecule 2: Heavy Chain of a VEGF binding Antibody



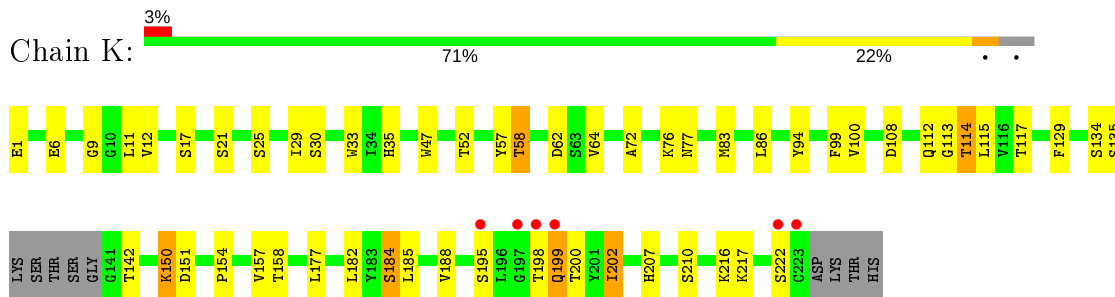
- Molecule 2: Heavy Chain of a VEGF binding Antibody



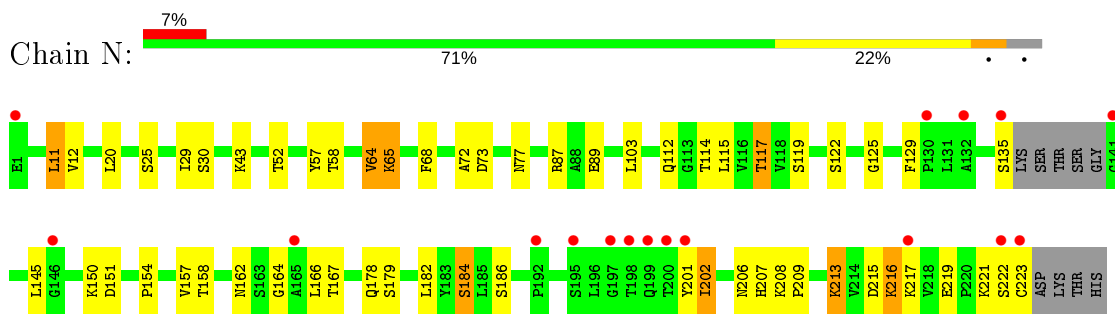
- Molecule 2: Heavy Chain of a VEGF binding Antibody



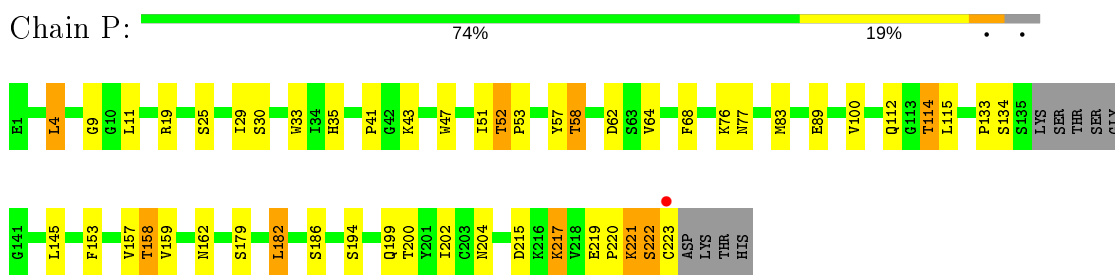
• Molecule 2: Heavy Chain of a VEGF binding Antibody



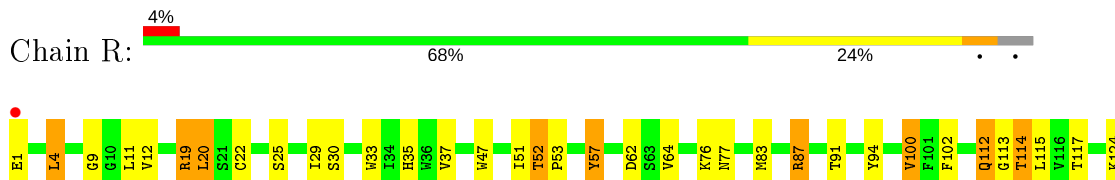
• Molecule 2: Heavy Chain of a VEGF binding Antibody

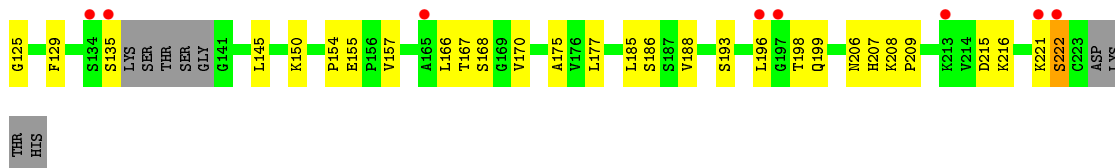


• Molecule 2: Heavy Chain of a VEGF binding Antibody

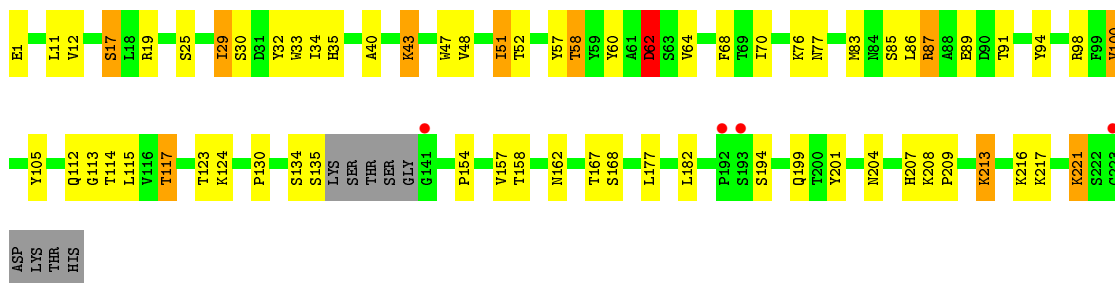


• Molecule 2: Heavy Chain of a VEGF binding Antibody

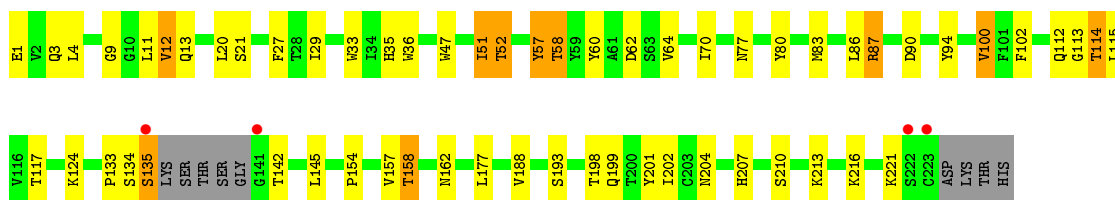




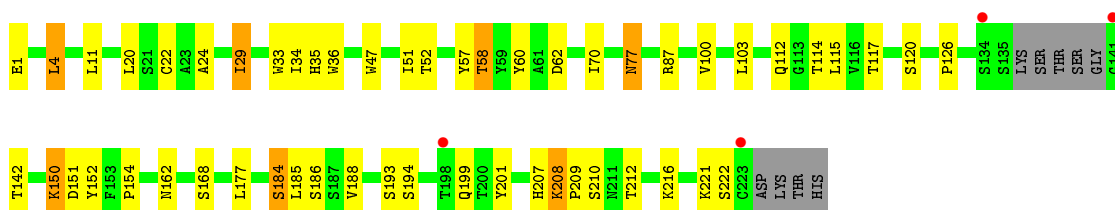
• Molecule 2: Heavy Chain of a VEGF binding Antibody



• Molecule 2: Heavy Chain of a VEGF binding Antibody



• Molecule 2: Heavy Chain of a VEGF binding Antibody



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	274.92Å 192.23Å 154.11Å 90.00° 117.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 29.96 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.65) 99.8 (29.96-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.64Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.248 0.194 , 0.241	Depositor DCC
R_{free} test set	4490 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	39642	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.41	0/1653	0.72	4/2248 (0.2%)
1	C	0.39	0/1653	0.75	7/2248 (0.3%)
1	E	0.39	0/1653	0.75	7/2248 (0.3%)
1	G	0.44	0/1653	0.75	3/2248 (0.1%)
1	J	0.44	0/1653	0.76	3/2248 (0.1%)
1	L	0.42	0/1653	0.72	5/2248 (0.2%)
1	M	0.42	0/1653	0.75	6/2248 (0.3%)
1	O	0.41	0/1653	0.75	5/2248 (0.2%)
1	Q	0.38	0/1653	0.72	6/2248 (0.3%)
1	S	0.37	0/1653	0.70	3/2248 (0.1%)
1	U	0.39	0/1653	0.72	5/2248 (0.2%)
1	W	0.39	0/1653	0.72	5/2248 (0.2%)
2	B	0.44	0/1677	0.73	0/2290
2	D	0.42	0/1677	0.74	4/2290 (0.2%)
2	F	0.42	0/1677	0.76	2/2290 (0.1%)
2	H	0.44	0/1677	0.76	2/2290 (0.1%)
2	I	0.48	0/1677	0.76	3/2290 (0.1%)
2	K	0.43	0/1677	0.73	3/2290 (0.1%)
2	N	0.42	0/1677	0.73	3/2290 (0.1%)
2	P	0.45	0/1677	0.75	3/2290 (0.1%)
2	R	0.42	0/1677	0.73	2/2290 (0.1%)
2	T	0.43	0/1677	0.73	1/2290 (0.0%)
2	V	0.42	0/1677	0.74	2/2290 (0.1%)
2	X	0.40	0/1677	0.71	2/2290 (0.1%)
All	All	0.42	0/39960	0.74	86/54456 (0.2%)

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	28	ASP	CB-CG-OD2	7.48	125.03	118.30
2	I	73	ASP	CB-CG-OD2	7.28	124.85	118.30
2	H	62	ASP	CB-CG-OD2	7.21	124.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	17	ASP	CB-CG-OD2	6.90	124.51	118.30
2	P	62	ASP	CB-CG-OD2	6.63	124.27	118.30
2	V	62	ASP	CB-CG-OD2	6.60	124.24	118.30
1	M	167	ASP	CB-CG-OD2	6.52	124.17	118.30
1	U	28	ASP	CB-CG-OD2	6.52	124.17	118.30
2	I	62	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	122	ASP	CB-CG-OD2	6.16	123.84	118.30
1	L	28	ASP	CB-CG-OD2	6.02	123.71	118.30
1	E	170	ASP	CB-CG-OD2	5.97	123.67	118.30
1	U	151	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	28	ASP	CB-CG-OD2	5.91	123.61	118.30
2	I	215	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	185	ASP	CB-CG-OD2	5.85	123.57	118.30
1	W	28	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	1	ASP	CB-CG-OD2	5.79	123.51	118.30
2	D	62	ASP	CB-CG-OD2	5.77	123.50	118.30
1	S	1	ASP	CB-CG-OD2	5.77	123.50	118.30
2	T	62	ASP	CB-CG-OD2	5.77	123.50	118.30
1	C	70	ASP	CB-CG-OD2	5.77	123.49	118.30
2	X	62	ASP	CB-CG-OD2	5.70	123.43	118.30
2	R	215	ASP	CB-CG-OD2	5.68	123.41	118.30
1	W	185	ASP	CB-CG-OD2	5.68	123.41	118.30
1	L	167	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	167	ASP	CB-CG-OD2	5.64	123.38	118.30
2	K	108	ASP	CB-CG-OD2	5.64	123.37	118.30
1	S	151	ASP	CB-CG-OD2	5.59	123.33	118.30
1	Q	28	ASP	CB-CG-OD2	5.58	123.33	118.30
1	O	28	ASP	CB-CG-OD2	5.56	123.31	118.30
1	Q	1	ASP	CB-CG-OD2	5.56	123.31	118.30
2	N	73	ASP	CB-CG-OD2	5.55	123.30	118.30
1	L	70	ASP	CB-CG-OD2	5.54	123.28	118.30
1	E	185	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	167	ASP	CB-CG-OD2	5.50	123.25	118.30
1	M	122	ASP	CB-CG-OD2	5.50	123.25	118.30
1	L	122	ASP	CB-CG-OD2	5.47	123.23	118.30
2	R	62	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	170	ASP	CB-CG-OD2	5.44	123.19	118.30
1	M	28	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	122	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	1	ASP	CB-CG-OD2	5.42	123.18	118.30
2	K	62	ASP	CB-CG-OD2	5.41	123.17	118.30
1	O	167	ASP	CB-CG-OD2	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	73	ASP	CB-CG-OD2	5.40	123.16	118.30
2	X	151	ASP	CB-CG-OD2	5.38	123.14	118.30
1	J	28	ASP	CB-CG-OD2	5.37	123.13	118.30
1	O	1	ASP	CB-CG-OD2	5.35	123.11	118.30
2	D	4	LEU	CA-CB-CG	5.33	127.55	115.30
2	V	90	ASP	CB-CG-OD2	5.32	123.08	118.30
1	G	28	ASP	CB-CG-OD2	5.31	123.08	118.30
2	N	215	ASP	CB-CG-OD2	5.30	123.07	118.30
1	S	122	ASP	CB-CG-OD2	5.30	123.07	118.30
1	M	170	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	82	ASP	CB-CG-OD2	5.29	123.06	118.30
1	G	167	ASP	CB-CG-OD2	5.29	123.06	118.30
2	P	215	ASP	CB-CG-OD2	5.28	123.06	118.30
1	M	82	ASP	CB-CG-OD2	5.28	123.05	118.30
1	J	185	ASP	CB-CG-OD2	5.27	123.05	118.30
1	G	1	ASP	CB-CG-OD2	5.27	123.04	118.30
1	W	122	ASP	CB-CG-OD2	5.25	123.03	118.30
2	P	4	LEU	CA-CB-CG	5.24	127.34	115.30
2	D	73	ASP	CB-CG-OD2	5.21	122.99	118.30
1	U	1	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	82	ASP	CB-CG-OD2	5.17	122.96	118.30
2	K	151	ASP	CB-CG-OD2	5.17	122.96	118.30
1	W	1	ASP	CB-CG-OD2	5.17	122.96	118.30
2	N	151	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	82	ASP	CB-CG-OD2	5.15	122.94	118.30
1	L	1	ASP	CB-CG-OD2	5.11	122.90	118.30
1	U	82	ASP	CB-CG-OD2	5.11	122.90	118.30
1	U	122	ASP	CB-CG-OD2	5.10	122.89	118.30
1	J	167	ASP	CB-CG-OD2	5.10	122.89	118.30
2	H	215	ASP	CB-CG-OD2	5.10	122.89	118.30
1	E	151	ASP	CB-CG-OD2	5.08	122.88	118.30
1	O	122	ASP	CB-CG-OD2	5.08	122.88	118.30
1	W	151	ASP	CB-CG-OD2	5.08	122.88	118.30
1	O	70	ASP	CB-CG-OD2	5.05	122.84	118.30
1	Q	151	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	185	ASP	CB-CG-OD2	5.04	122.83	118.30
1	Q	70	ASP	CB-CG-OD2	5.03	122.83	118.30
1	Q	122	ASP	CB-CG-OD2	5.02	122.82	118.30
2	F	215	ASP	CB-CG-OD2	5.02	122.82	118.30
1	M	185	ASP	CB-CG-OD2	5.02	122.82	118.30
2	D	31	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1617	0	1573	25	0
1	C	1617	0	1573	13	0
1	E	1617	0	1573	14	0
1	G	1617	0	1573	23	0
1	J	1617	0	1573	14	0
1	L	1617	0	1573	15	0
1	M	1617	0	1573	21	0
1	O	1617	0	1573	22	0
1	Q	1617	0	1573	19	0
1	S	1617	0	1573	26	0
1	U	1617	0	1573	26	0
1	W	1617	0	1573	16	0
2	B	1633	0	1592	17	0
2	D	1633	0	1592	12	0
2	F	1633	0	1592	21	0
2	H	1633	0	1592	26	0
2	I	1633	0	1592	30	0
2	K	1633	0	1592	23	0
2	N	1633	0	1592	28	0
2	P	1633	0	1592	19	0
2	R	1633	0	1592	28	0
2	T	1633	0	1592	32	0
2	V	1633	0	1592	33	0
2	X	1633	0	1592	22	0
3	A	17	0	0	1	0
3	B	28	0	0	0	0
3	C	10	0	0	0	0
3	D	30	0	0	0	0
3	E	14	0	0	0	0
3	F	30	0	0	2	0
3	G	53	0	0	3	0
3	H	44	0	0	3	0
3	I	52	0	0	2	0
3	J	35	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	53	0	0	2	0
3	L	22	0	0	0	0
3	M	17	0	0	1	0
3	N	24	0	0	0	0
3	O	31	0	0	3	0
3	P	52	0	0	2	0
3	Q	15	0	0	0	0
3	R	21	0	0	1	0
3	S	9	0	0	1	0
3	T	15	0	0	2	0
3	U	16	0	0	2	0
3	V	28	0	0	2	0
3	W	5	0	0	0	0
3	X	21	0	0	1	0
All	All	39642	0	37980	508	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (508) 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)
2:R:19:ARG:HH11	2:R:19:ARG:HG3	1.22	0.99
1:S:83:PHE:CE1	1:S:106:ILE:HD11	2.00	0.96
2:X:35:HIS:HD2	2:X:47:TRP:HE1	1.13	0.93
2:I:52:THR:HG21	3:I:265:HOH:O	1.72	0.90
1:E:83:PHE:HZ	1:E:165:GLU:HG2	1.39	0.86
1:C:40:PRO:HG3	1:C:165:GLU:HG2	1.58	0.86
1:C:183:LYS:O	1:C:187:GLU:HG2	1.77	0.84
2:P:162:ASN:HD21	2:P:202:ILE:H	1.25	0.84
2:I:13:GLN:HG3	2:N:213:LYS:HD3	1.58	0.83
2:F:58:THR:HG21	3:F:230:HOH:O	1.80	0.82
2:N:29:ILE:HG13	2:N:77:ASN:OD1	1.78	0.81
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.26	0.80
1:J:39:LYS:HE3	3:J:240:HOH:O	1.82	0.79
1:M:160:GLN:HE22	2:N:178:GLN:HA	1.47	0.79
2:X:35:HIS:CD2	2:X:47:TRP:HE1	1.99	0.79
2:K:29:ILE:HG13	2:K:77:ASN:ND2	1.99	0.78
2:R:35:HIS:CD2	2:R:47:TRP:HE1	2.03	0.76
2:X:58:THR:HG21	3:X:235:HOH:O	1.84	0.76
2:P:162:ASN:ND2	2:P:202:ILE:H	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:126:PRO:HB3	2:X:152:TYR:HB3	1.68	0.76
1:S:90:GLN:NE2	1:S:93:THR:H	1.82	0.76
2:B:154:PRO:O	2:B:207:HIS:HE1	1.69	0.75
2:H:13:GLN:H	2:H:13:GLN:HE21	1.33	0.74
2:R:29:ILE:HG13	2:R:77:ASN:ND2	2.02	0.74
2:T:29:ILE:HG13	2:T:77:ASN:ND2	2.02	0.74
2:H:154:PRO:O	2:H:207:HIS:HE1	1.70	0.74
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.05	0.74
2:P:58:THR:HG21	3:P:231:HOH:O	1.87	0.74
1:G:1:ASP:N	1:G:1:ASP:OD1	2.21	0.73
2:T:34:ILE:HB	2:T:51:ILE:HD11	1.69	0.73
2:D:150:LYS:HA	2:D:184:SER:HB2	1.71	0.72
1:S:90:GLN:HE21	1:S:93:THR:H	1.37	0.72
2:V:35:HIS:CD2	2:V:47:TRP:HE1	2.08	0.71
1:O:164:THR:HG22	1:O:174:SER:H	1.54	0.71
2:I:13:GLN:HG3	2:N:213:LYS:CD	2.21	0.71
1:L:164:THR:HG23	1:L:165:GLU:O	1.90	0.71
1:L:198:HIS:CD2	1:L:200:GLY:H	2.08	0.70
2:N:206:ASN:ND2	2:N:213:LYS:HG3	2.07	0.70
1:J:198:HIS:CD2	1:J:200:GLY:H	2.09	0.69
1:U:147:GLN:HG2	1:U:154:LEU:HD11	1.75	0.69
1:A:183:LYS:O	1:A:187:GLU:HG2	1.92	0.69
1:G:198:HIS:CD2	1:G:200:GLY:H	2.12	0.68
1:W:14:SER:O	1:W:17:ASP:HB2	1.94	0.68
1:A:108:ARG:HD3	1:A:109:THR:O	1.94	0.67
2:T:154:PRO:O	2:T:207:HIS:HE1	1.78	0.67
2:D:154:PRO:O	2:D:207:HIS:HE1	1.77	0.67
2:I:35:HIS:HD2	2:I:47:TRP:HE1	1.39	0.66
1:W:161:GLU:HG2	1:W:175:LEU:HD21	1.77	0.66
2:X:35:HIS:HD2	2:X:47:TRP:NE1	1.90	0.66
2:H:117:THR:HG22	3:H:253:HOH:O	1.95	0.66
2:I:35:HIS:CD2	2:I:47:TRP:HE1	2.13	0.66
2:T:58:THR:HG21	3:T:235:HOH:O	1.94	0.66
2:P:200:THR:HG23	2:P:217:LYS:HE3	1.77	0.66
2:R:19:ARG:NH1	2:R:19:ARG:HG3	1.98	0.65
1:S:83:PHE:CZ	1:S:106:ILE:HD11	2.31	0.65
1:U:198:HIS:CD2	1:U:200:GLY:H	2.14	0.65
2:I:162:ASN:ND2	2:I:202:ILE:H	1.95	0.65
1:A:186:TYR:CE2	1:A:211:ARG:HD2	2.32	0.65
1:Q:21:ILE:HG12	1:Q:102:THR:HG21	1.77	0.65
2:V:29:ILE:HG13	2:V:77:ASN:ND2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:198:HIS:CD2	1:S:200:GLY:H	2.16	0.64
3:A:220:HOH:O	2:F:58:THR:HG22	1.97	0.64
1:Q:147:GLN:HB3	1:Q:195:GLU:HB3	1.77	0.64
1:U:45:LYS:NZ	3:U:224:HOH:O	2.29	0.64
2:X:29:ILE:HG13	2:X:77:ASN:ND2	2.12	0.64
1:O:1:ASP:N	3:O:234:HOH:O	2.29	0.64
2:X:207:HIS:HD2	2:X:210:SER:OG	1.81	0.64
2:T:34:ILE:HB	2:T:51:ILE:CD1	2.27	0.63
2:P:29:ILE:HG13	2:P:77:ASN:ND2	2.12	0.63
2:V:154:PRO:O	2:V:207:HIS:HE1	1.80	0.63
2:P:35:HIS:CD2	2:P:47:TRP:HE1	2.17	0.63
2:N:206:ASN:HD22	2:N:213:LYS:HE2	1.63	0.63
2:V:12:VAL:HG21	2:V:86:LEU:HD13	1.80	0.63
2:F:34:ILE:HB	2:F:51:ILE:HD11	1.81	0.62
2:X:154:PRO:O	2:X:207:HIS:HE1	1.83	0.62
2:V:87:ARG:HG3	2:V:87:ARG:HH11	1.63	0.62
1:L:155:GLN:HB3	1:L:158:ASN:HD21	1.65	0.62
2:V:51:ILE:HG13	2:V:70:ILE:CD1	2.30	0.62
1:E:83:PHE:CZ	1:E:165:GLU:HG2	2.29	0.62
2:P:153:PHE:HB2	2:P:182:LEU:HD12	1.81	0.62
2:V:133:PRO:HG3	2:V:145:LEU:HB3	1.82	0.62
1:A:10:SER:HB2	1:A:103:LYS:HB2	1.82	0.61
1:W:198:HIS:CD2	1:W:200:GLY:H	2.17	0.61
2:N:154:PRO:O	2:N:207:HIS:HE1	1.83	0.61
2:K:35:HIS:CD2	2:K:47:TRP:HE1	2.19	0.61
2:H:58:THR:HG21	3:H:234:HOH:O	2.00	0.61
2:H:207:HIS:HD2	2:H:210:SER:OG	1.83	0.60
2:V:35:HIS:HD2	2:V:47:TRP:HE1	1.48	0.60
1:E:198:HIS:CD2	1:E:200:GLY:H	2.20	0.60
2:V:207:HIS:HD2	2:V:210:SER:OG	1.85	0.59
2:I:154:PRO:O	2:I:207:HIS:HE1	1.84	0.59
2:V:87:ARG:HG3	2:V:87:ARG:NH1	2.17	0.59
2:F:154:PRO:O	2:F:207:HIS:HE1	1.85	0.59
1:W:134:CYS:HB2	1:W:148:TRP:CZ2	2.37	0.59
1:O:164:THR:HG23	1:O:165:GLU:O	2.02	0.59
2:B:58:THR:HG23	2:B:60:TYR:CE1	2.38	0.59
2:H:202:ILE:HD12	2:H:204:ASN:HD21	1.65	0.59
1:G:164:THR:HG22	1:G:174:SER:H	1.68	0.59
1:E:186:TYR:HA	1:E:192:TYR:OH	2.03	0.59
2:N:29:ILE:HD12	2:N:30:SER:H	1.67	0.58
1:U:143:GLU:CD	1:U:143:GLU:H	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:134:SER:O	2:V:135:SER:HB2	2.01	0.58
2:B:33:TRP:HA	2:B:51:ILE:O	2.03	0.58
2:N:162:ASN:ND2	2:N:202:ILE:H	2.01	0.58
2:F:117:THR:CG2	3:F:257:HOH:O	2.52	0.58
2:V:94:TYR:O	2:V:113:GLY:HA2	2.04	0.58
2:K:35:HIS:HD2	2:K:47:TRP:HE1	1.52	0.57
2:P:9:GLY:H	2:P:114:THR:HG21	1.69	0.57
1:L:161:GLU:HG2	1:L:175:LEU:HD21	1.87	0.57
1:U:158:ASN:N	1:U:158:ASN:HD22	2.03	0.57
2:H:221:LYS:HD2	2:H:222:SER:H	1.68	0.57
1:Q:198:HIS:CD2	1:Q:200:GLY:H	2.23	0.57
2:V:51:ILE:HG13	2:V:70:ILE:HD13	1.87	0.57
1:C:108:ARG:HG2	1:C:171:SER:HB2	1.87	0.56
1:J:198:HIS:HB3	1:J:201:LEU:HD22	1.86	0.56
2:I:52:THR:HG23	2:I:53:PRO:HD2	1.86	0.56
2:I:207:HIS:HD2	2:I:210:SER:OG	1.88	0.56
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.88	0.56
1:S:164:THR:HG22	1:S:174:SER:H	1.70	0.56
1:G:29:VAL:HG11	1:G:90:GLN:HG3	1.87	0.56
2:H:117:THR:CG2	3:H:253:HOH:O	2.52	0.56
2:P:158:THR:HG22	3:P:267:HOH:O	2.06	0.56
1:A:198:HIS:CD2	1:A:200:GLY:H	2.24	0.56
2:K:207:HIS:HD2	2:K:210:SER:OG	1.89	0.56
1:A:123:GLU:HA	1:A:126:LYS:NZ	2.21	0.56
1:S:83:PHE:CD1	1:S:106:ILE:HD11	2.40	0.56
2:X:36:TRP:HD1	2:X:70:ILE:HD12	1.71	0.56
2:V:51:ILE:HG12	2:V:70:ILE:HG12	1.88	0.55
1:M:185:ASP:HA	1:M:188:LYS:HE2	1.88	0.55
2:P:35:HIS:HD2	2:P:47:TRP:HE1	1.53	0.55
2:I:62:ASP:N	2:I:62:ASP:OD1	2.38	0.55
1:M:83:PHE:O	1:M:83:PHE:CD2	2.59	0.55
2:I:162:ASN:HD21	2:I:202:ILE:H	1.53	0.55
1:G:112:ALA:HB1	1:G:201:LEU:HD13	1.88	0.55
1:O:198:HIS:CD2	1:O:200:GLY:H	2.24	0.55
2:V:58:THR:HG21	3:V:248:HOH:O	2.07	0.55
1:Q:121:SER:OG	2:R:129:PHE:HB3	2.07	0.55
2:F:52:THR:HB	2:F:57:TYR:H	1.70	0.55
2:N:150:LYS:HA	2:N:184:SER:HB2	1.89	0.55
1:W:140:TYR:CG	1:W:141:PRO:HA	2.41	0.55
2:T:17:SER:HA	2:T:83:MET:O	2.07	0.54
1:G:24:ARG:HD3	1:G:70:ASP:OD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:29:ILE:HG13	2:I:77:ASN:OD1	2.08	0.54
2:K:58:THR:HG21	3:K:259:HOH:O	2.08	0.54
2:H:202:ILE:HA	2:H:216:LYS:O	2.07	0.54
2:H:29:ILE:HG13	2:H:77:ASN:ND2	2.22	0.54
1:A:6:GLN:NE2	1:A:86:TYR:O	2.40	0.54
1:G:165:GLU:HG2	3:G:263:HOH:O	2.07	0.54
1:M:198:HIS:CD2	1:M:200:GLY:H	2.26	0.54
2:R:29:ILE:HD12	2:R:30:SER:N	2.23	0.54
2:R:154:PRO:O	2:R:207:HIS:HE1	1.90	0.54
2:B:162:ASN:ND2	2:B:202:ILE:H	2.05	0.54
1:Q:100:GLN:H	1:Q:100:GLN:NE2	2.06	0.54
2:T:58:THR:HG23	2:T:60:TYR:CE1	2.43	0.54
1:J:198:HIS:HD2	1:J:200:GLY:H	1.53	0.53
1:U:29:VAL:HG11	1:U:90:GLN:HG3	1.90	0.53
1:O:47:LEU:HA	1:O:58:VAL:HG21	1.90	0.53
1:M:36:TYR:HE2	1:M:89:GLN:HE21	1.57	0.53
1:Q:121:SER:O	1:Q:125:LEU:HD22	2.08	0.53
2:V:83:MET:HB3	2:V:86:LEU:HD21	1.91	0.53
2:X:162:ASN:HD21	2:X:201:TYR:HA	1.73	0.53
1:L:103:LYS:HD2	1:L:105:GLU:OE2	2.09	0.53
2:R:35:HIS:HD2	2:R:47:TRP:HE1	1.51	0.53
1:L:29:VAL:HG11	1:L:90:GLN:HG3	1.89	0.53
2:P:133:PRO:HG3	2:P:145:LEU:HB3	1.91	0.53
2:V:158:THR:HG22	3:V:244:HOH:O	2.09	0.53
1:C:164:THR:HG23	1:C:165:GLU:O	2.09	0.53
2:X:126:PRO:HD2	2:X:212:THR:HG21	1.91	0.53
2:V:51:ILE:CG1	2:V:70:ILE:HG12	2.39	0.52
1:U:120:PRO:HD3	1:U:132:VAL:HG22	1.91	0.52
1:W:134:CYS:HB2	1:W:148:TRP:CH2	2.44	0.52
2:F:64:VAL:HG13	2:F:68:PHE:HB2	1.92	0.52
2:K:29:ILE:HD12	2:K:30:SER:H	1.73	0.52
2:V:9:GLY:H	2:V:114:THR:HG21	1.74	0.52
1:W:183:LYS:O	1:W:187:GLU:HG2	2.09	0.52
1:S:11:LEU:HD13	1:S:19:VAL:HG21	1.92	0.52
2:I:157:VAL:HG12	2:I:185:LEU:HD21	1.91	0.52
2:F:100:VAL:HG13	2:F:102:PHE:HB2	1.91	0.52
2:N:206:ASN:ND2	2:N:213:LYS:CG	2.72	0.52
2:D:207:HIS:HD2	2:D:210:SER:OG	1.93	0.52
1:A:36:TYR:HE2	1:A:89:GLN:HE21	1.58	0.52
1:G:36:TYR:OH	1:G:89:GLN:NE2	2.43	0.51
2:T:51:ILE:HG13	2:T:70:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:TYR:O	2:B:113:GLY:HA2	2.11	0.51
2:D:29:ILE:HD12	2:D:30:SER:H	1.75	0.51
2:K:29:ILE:HD12	2:K:30:SER:N	2.25	0.51
1:U:164:THR:HG22	1:U:174:SER:H	1.76	0.51
1:U:164:THR:HG23	1:U:165:GLU:O	2.10	0.51
1:A:83:PHE:C	1:A:83:PHE:CD2	2.83	0.51
1:O:54:LEU:HD21	1:O:60:SER:HA	1.93	0.51
1:A:141:PRO:O	1:A:198:HIS:HE1	1.94	0.51
2:D:29:ILE:HG13	2:D:77:ASN:OD1	2.11	0.51
2:F:211:ASN:O	2:V:13:GLN:NE2	2.43	0.51
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.94	0.51
1:A:140:TYR:CG	1:A:141:PRO:HA	2.46	0.50
2:B:102:PHE:CD2	2:F:72:ALA:HB3	2.47	0.50
1:G:20:THR:HG22	1:G:74:THR:HG23	1.92	0.50
1:O:209:PHE:C	1:O:210:ASN:HD22	2.14	0.50
2:H:13:GLN:H	2:H:13:GLN:NE2	2.06	0.50
2:K:29:ILE:H	2:K:77:ASN:HD21	1.59	0.50
1:W:114:SER:HB2	1:W:137:ASN:HB3	1.93	0.50
2:D:33:TRP:HA	2:D:51:ILE:O	2.11	0.50
1:J:20:THR:HG22	1:J:74:THR:HG23	1.94	0.50
1:M:164:THR:HG23	1:M:165:GLU:O	2.11	0.50
1:O:4:MET:SD	1:O:90:GLN:HB2	2.52	0.50
1:A:117:ILE:HD12	1:A:194:CYS:HB3	1.93	0.50
2:H:207:HIS:CD2	2:H:210:SER:OG	2.64	0.50
2:V:33:TRP:HA	2:V:51:ILE:O	2.11	0.50
2:T:29:ILE:HD12	2:T:30:SER:H	1.77	0.50
2:V:4:LEU:HD21	2:V:27:PHE:HZ	1.77	0.50
2:X:150:LYS:HA	2:X:184:SER:HB2	1.93	0.50
2:H:100:VAL:HG13	2:H:102:PHE:H	1.76	0.50
2:F:165:ALA:O	1:W:18:ARG:NH2	2.45	0.49
2:F:36:TRP:HD1	2:F:70:ILE:HD12	1.77	0.49
2:I:58:THR:HG21	3:I:231:HOH:O	2.11	0.49
1:S:35:TRP:CZ3	1:S:88:CYS:HB3	2.47	0.49
2:N:11:LEU:HD23	2:N:117:THR:O	2.11	0.49
2:V:52:THR:HB	2:V:57:TYR:H	1.76	0.49
1:W:21:ILE:HG12	1:W:102:THR:HG21	1.93	0.49
1:G:123:GLU:O	1:G:126:LYS:HB2	2.13	0.49
1:S:133:VAL:HG22	1:S:178:THR:HG23	1.95	0.49
1:U:158:ASN:H	1:U:158:ASN:HD22	1.60	0.49
2:B:34:ILE:HB	2:B:51:ILE:HD11	1.94	0.49
1:M:29:VAL:HG11	1:M:90:GLN:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:87:ARG:HG3	2:T:87:ARG:NH1	2.27	0.49
1:U:140:TYR:CG	1:U:141:PRO:HA	2.47	0.49
2:X:208:LYS:N	2:X:209:PRO:CD	2.76	0.49
2:T:51:ILE:HG13	2:T:70:ILE:CD1	2.42	0.49
2:K:9:GLY:H	2:K:114:THR:HG21	1.77	0.49
2:P:89:GLU:H	2:P:89:GLU:CD	2.16	0.49
1:S:183:LYS:HG3	1:S:187:GLU:HG3	1.95	0.49
2:F:87:ARG:HD3	2:F:89:GLU:OE2	2.12	0.49
2:I:161:TRP:HB3	2:I:166:LEU:HD23	1.95	0.49
2:R:20:LEU:HD22	2:R:83:MET:SD	2.52	0.49
2:B:162:ASN:HD21	2:B:202:ILE:H	1.61	0.48
1:Q:14:SER:O	1:Q:17:ASP:HB2	2.14	0.48
2:T:32:TYR:CD2	2:T:98:ARG:HD2	2.47	0.48
1:L:182:SER:OG	1:L:185:ASP:HB2	2.13	0.48
2:R:112:GLN:HG3	3:R:247:HOH:O	2.14	0.48
1:U:183:LYS:O	1:U:187:GLU:HG2	2.13	0.48
2:F:40:ALA:HB3	2:F:43:LYS:HD2	1.95	0.48
2:R:29:ILE:HD12	2:R:30:SER:H	1.77	0.48
2:R:87:ARG:CG	2:R:87:ARG:HH11	2.27	0.48
2:X:35:HIS:CD2	2:X:47:TRP:NE1	2.74	0.48
1:G:141:PRO:O	1:G:198:HIS:HE1	1.96	0.48
1:M:135:LEU:HD22	1:M:136:LEU:H	1.78	0.48
2:R:91:THR:HG23	2:R:117:THR:HA	1.94	0.48
2:T:34:ILE:H	2:T:51:ILE:HD12	1.79	0.48
1:U:161:GLU:HG2	1:U:175:LEU:HD21	1.96	0.48
1:G:19:VAL:HG11	1:G:78:LEU:HD13	1.96	0.48
1:O:164:THR:CG2	1:O:174:SER:H	2.24	0.48
1:O:39:LYS:NZ	1:O:81:GLU:O	2.46	0.48
2:R:87:ARG:CB	2:R:87:ARG:HH11	2.26	0.48
2:T:33:TRP:HA	2:T:51:ILE:O	2.13	0.48
2:V:12:VAL:HG21	2:V:86:LEU:CD1	2.44	0.48
2:N:29:ILE:HD12	2:N:30:SER:N	2.28	0.48
1:W:6:GLN:OE1	1:W:99:GLY:HA3	2.14	0.48
2:F:207:HIS:HD2	2:F:210:SER:OG	1.96	0.48
1:G:164:THR:CG2	3:G:225:HOH:O	2.62	0.48
1:A:108:ARG:HG2	1:A:171:SER:HB3	1.96	0.48
2:K:150:LYS:HA	2:K:184:SER:OG	2.14	0.48
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.95	0.48
2:T:162:ASN:HD21	2:T:201:TYR:HA	1.79	0.48
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.49	0.47
1:J:181:LEU:HD13	1:J:186:TYR:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4:MET:SD	1:J:90:GLN:HB2	2.54	0.47
2:K:94:TYR:O	2:K:113:GLY:HA2	2.14	0.47
2:T:154:PRO:HD2	2:T:209:PRO:HB2	1.96	0.47
2:I:2:VAL:HG13	2:I:27:PHE:CD1	2.50	0.47
2:N:208:LYS:HB3	2:N:209:PRO:HD3	1.95	0.47
2:V:58:THR:HG23	2:V:60:TYR:CE1	2.50	0.47
1:C:187:GLU:HA	1:C:211:ARG:NH2	2.29	0.47
2:K:150:LYS:HG2	2:K:184:SER:OG	2.15	0.47
1:M:129:THR:HB	1:M:181:LEU:O	2.14	0.47
2:P:33:TRP:HA	2:P:51:ILE:O	2.15	0.47
2:I:153:PHE:HB2	2:I:182:LEU:HD12	1.96	0.47
2:I:4:LEU:HD21	2:I:27:PHE:HZ	1.79	0.47
1:C:24:ARG:HG3	1:C:24:ARG:O	2.14	0.47
2:H:58:THR:HG23	2:H:60:TYR:CE1	2.50	0.47
2:K:157:VAL:CG1	2:K:185:LEU:HD21	2.45	0.47
1:L:83:PHE:CD1	1:L:83:PHE:C	2.87	0.47
2:V:21:SER:HB3	2:V:80:TYR:CD1	2.50	0.47
2:V:87:ARG:HH11	2:V:87:ARG:CG	2.28	0.47
2:I:33:TRP:HA	2:I:51:ILE:O	2.13	0.47
2:K:154:PRO:O	2:K:207:HIS:HE1	1.97	0.47
1:O:197:THR:HG23	1:O:204:PRO:HG3	1.97	0.47
1:L:198:HIS:HD2	1:L:200:GLY:H	1.59	0.47
1:M:36:TYR:OH	1:M:89:GLN:NE2	2.48	0.47
1:O:164:THR:CG2	3:O:227:HOH:O	2.63	0.47
1:U:124:GLN:HE22	1:U:131:SER:HB2	1.78	0.47
1:J:121:SER:OG	2:K:129:PHE:HB3	2.14	0.47
1:A:3:GLN:HG3	1:A:26:SER:HB3	1.97	0.47
1:E:83:PHE:HZ	1:E:165:GLU:CG	2.18	0.47
1:S:164:THR:HG23	1:S:165:GLU:O	2.15	0.47
2:T:48:VAL:HG13	2:T:64:VAL:HG21	1.96	0.47
1:C:83:PHE:HZ	1:C:165:GLU:CG	2.27	0.46
2:T:62:ASP:N	2:T:62:ASP:OD2	2.47	0.46
2:X:207:HIS:CD2	2:X:210:SER:OG	2.66	0.46
2:F:91:THR:HG23	2:F:117:THR:HA	1.98	0.46
1:M:135:LEU:HD22	1:M:136:LEU:N	2.30	0.46
2:D:83:MET:HE2	2:D:86:LEU:HD21	1.97	0.46
1:Q:6:GLN:H	1:Q:100:GLN:HE22	1.62	0.46
1:O:108:ARG:HD3	1:O:109:THR:O	2.16	0.46
2:P:29:ILE:HD12	2:P:30:SER:H	1.80	0.46
1:A:20:THR:HG22	1:A:74:THR:OG1	2.16	0.46
2:D:102:PHE:CD2	2:K:72:ALA:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:VAL:HG13	2:D:68:PHE:HB2	1.97	0.46
2:V:100:VAL:HG13	2:V:102:PHE:HB2	1.98	0.46
2:T:94:TYR:O	2:T:113:GLY:HA2	2.15	0.46
2:B:12:VAL:HG21	2:B:86:LEU:HD13	1.98	0.46
1:M:24:ARG:HB2	1:M:24:ARG:HE	1.54	0.46
2:I:211:ASN:CB	2:N:11:LEU:HD13	2.46	0.46
1:S:47:LEU:HA	1:S:58:VAL:HG21	1.98	0.46
1:C:198:HIS:CD2	1:C:200:GLY:H	2.34	0.46
2:N:206:ASN:ND2	2:N:213:LYS:HE2	2.29	0.46
1:O:151:ASP:O	1:O:152:ASN:HB2	2.14	0.46
1:S:1:ASP:HB3	3:S:217:HOH:O	2.15	0.46
2:T:87:ARG:HH11	2:T:87:ARG:HG3	1.80	0.46
1:Q:2:ILE:HG12	1:Q:27:GLN:HG3	1.98	0.46
2:R:175:ALA:HA	2:R:185:LEU:HB3	1.97	0.46
1:E:185:ASP:HA	1:E:188:LYS:HD2	1.98	0.45
1:U:37:GLN:HB2	1:U:47:LEU:HD11	1.97	0.45
1:U:143:GLU:CD	1:U:143:GLU:N	2.70	0.45
1:C:83:PHE:CZ	1:C:165:GLU:HG3	2.51	0.45
2:H:29:ILE:HD12	2:H:30:SER:N	2.32	0.45
1:O:164:THR:HG21	3:O:227:HOH:O	2.16	0.45
1:W:18:ARG:HE	1:W:74:THR:HG21	1.80	0.45
1:A:4:MET:SD	1:A:90:GLN:HB2	2.56	0.45
2:K:6:GLU:HA	2:K:21:SER:O	2.16	0.45
2:H:94:TYR:O	2:H:113:GLY:HA2	2.15	0.45
1:O:198:HIS:HB3	1:O:201:LEU:HD22	1.98	0.45
1:S:23:CYS:HB2	1:S:35:TRP:CH2	2.50	0.45
1:S:159:SER:HA	1:S:178:THR:O	2.17	0.45
2:F:29:ILE:HD12	2:F:30:SER:H	1.81	0.45
2:X:33:TRP:HA	2:X:51:ILE:O	2.17	0.45
1:A:198:HIS:HB3	1:A:201:LEU:HD22	1.98	0.45
2:B:73:ASP:HB2	2:N:103:LEU:HD12	1.98	0.45
2:I:38:ARG:HD3	2:I:48:VAL:HG21	1.99	0.45
1:O:21:ILE:HG12	1:O:102:THR:HG21	1.97	0.45
2:B:178:GLN:HB2	2:B:182:LEU:O	2.18	0.44
1:G:198:HIS:HD2	1:G:200:GLY:H	1.64	0.44
1:J:151:ASP:O	1:J:152:ASN:HB2	2.17	0.44
2:T:40:ALA:HB3	2:T:43:LYS:HD3	1.98	0.44
1:U:117:ILE:HG12	1:U:209:PHE:HD2	1.82	0.44
1:G:37:GLN:HB2	1:G:47:LEU:HD11	1.99	0.44
1:J:199:GLN:HB2	3:J:249:HOH:O	2.17	0.44
1:M:124:GLN:HG3	2:N:129:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:VAL:HG13	2:B:68:PHE:HB2	2.00	0.44
2:H:52:THR:HG23	2:H:53:PRO:HD2	1.99	0.44
2:I:126:PRO:HB3	2:I:152:TYR:HB3	1.98	0.44
2:X:4:LEU:HG	2:X:22:CYS:SG	2.57	0.44
2:B:36:TRP:HD1	2:B:70:ILE:HD12	1.82	0.44
1:E:193:ALA:HB2	1:E:208:SER:HB3	1.98	0.44
2:N:162:ASN:HD21	2:N:201:TYR:HA	1.82	0.44
1:S:142:ARG:NH1	1:S:163:VAL:HG21	2.33	0.44
1:U:108:ARG:HD3	1:U:109:THR:O	2.17	0.44
1:U:47:LEU:HA	1:U:58:VAL:HG21	2.00	0.44
2:K:202:ILE:HG13	2:K:217:LYS:HA	1.99	0.44
2:P:159:VAL:HA	2:P:204:ASN:O	2.17	0.44
2:R:87:ARG:HB2	2:R:87:ARG:HH11	1.83	0.44
1:Q:181:LEU:HD13	1:Q:185:ASP:HB3	2.00	0.44
1:Q:22:THR:HG22	1:Q:72:THR:HG22	2.00	0.44
2:B:2:VAL:HG13	2:B:27:PHE:CD1	2.53	0.44
1:G:39:LYS:NZ	1:G:81:GLU:O	2.51	0.44
1:Q:29:VAL:HG11	1:Q:90:GLN:HG3	1.98	0.44
1:S:121:SER:HB2	2:T:130:PRO:HD2	1.99	0.44
1:S:37:GLN:HB2	1:S:47:LEU:HD11	2.00	0.44
1:U:198:HIS:HD2	1:U:200:GLY:H	1.65	0.44
1:A:143:GLU:CD	1:A:143:GLU:H	2.20	0.43
1:Q:106:ILE:H	1:Q:166:GLN:HE22	1.66	0.43
2:I:162:ASN:HD21	2:I:201:TYR:HA	1.84	0.43
2:X:207:HIS:HB3	2:X:212:THR:HB	1.99	0.43
1:Q:118:PHE:HB2	1:Q:133:VAL:HB	2.00	0.43
1:U:142:ARG:HG2	1:U:142:ARG:NH1	2.33	0.43
1:C:37:GLN:HB2	1:C:47:LEU:HD11	2.01	0.43
1:J:21:ILE:HG12	1:J:102:THR:HG21	2.01	0.43
2:R:208:LYS:N	2:R:209:PRO:CD	2.81	0.43
1:S:89:GLN:HE21	1:S:89:GLN:HB3	1.62	0.43
1:U:121:SER:OG	1:U:124:GLN:HB2	2.19	0.43
2:H:28:THR:HA	2:H:77:ASN:HD21	1.84	0.43
2:I:178:GLN:C	2:I:180:SER:H	2.21	0.43
1:L:163:VAL:HG22	1:L:175:LEU:HD12	2.01	0.43
1:S:94:THR:HG21	2:T:33:TRP:CH2	2.53	0.43
2:I:211:ASN:HB2	2:N:11:LEU:HD13	1.99	0.43
2:N:162:ASN:C	2:N:164:GLY:H	2.21	0.43
1:Q:164:THR:HG22	1:Q:173:TYR:HA	1.99	0.43
2:R:94:TYR:O	2:R:113:GLY:HA2	2.19	0.43
2:X:58:THR:HG23	2:X:60:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:SER:HA	1:A:178:THR:O	2.19	0.43
2:K:158:THR:HG22	3:K:271:HOH:O	2.18	0.43
2:T:64:VAL:HG13	2:T:68:PHE:HB2	1.99	0.43
2:I:91:THR:HG23	2:I:117:THR:HA	2.00	0.43
2:N:65:LYS:HE2	2:N:65:LYS:HB2	1.84	0.43
1:M:121:SER:O	1:M:125:LEU:HD13	2.19	0.43
2:F:102:PHE:CD1	2:N:72:ALA:HB3	2.54	0.43
1:G:140:TYR:CG	1:G:141:PRO:HA	2.54	0.43
1:G:207:LYS:HD3	1:G:207:LYS:HA	1.82	0.43
1:G:186:TYR:CZ	1:G:211:ARG:HG3	2.54	0.43
2:P:68:PHE:CZ	2:P:83:MET:HE2	2.53	0.43
1:W:133:VAL:HG22	1:W:178:THR:HG23	1.99	0.43
1:G:164:THR:HG21	3:G:225:HOH:O	2.18	0.42
2:X:29:ILE:HG13	2:X:29:ILE:H	1.63	0.42
2:H:208:LYS:N	2:H:209:PRO:CD	2.82	0.42
1:J:37:GLN:HB2	1:J:47:LEU:HD11	2.01	0.42
2:N:162:ASN:HD21	2:N:202:ILE:H	1.66	0.42
1:O:106:ILE:HG13	1:O:107:LYS:N	2.34	0.42
2:R:124:LYS:HE3	2:R:125:GLY:O	2.19	0.42
1:S:198:HIS:HD2	1:S:200:GLY:H	1.66	0.42
2:V:60:TYR:HB3	2:V:64:VAL:HG12	2.01	0.42
1:C:108:ARG:O	1:C:109:THR:O	2.37	0.42
1:M:35:TRP:CZ3	1:M:88:CYS:HB3	2.54	0.42
1:S:106:ILE:HA	1:S:106:ILE:HD13	1.60	0.42
1:S:160:GLN:HB2	1:S:160:GLN:HE21	1.67	0.42
1:L:108:ARG:HD3	1:L:109:THR:O	2.19	0.42
2:H:162:ASN:HA	2:H:202:ILE:HG13	2.00	0.42
2:H:35:HIS:CD2	2:H:47:TRP:NE1	2.82	0.42
2:R:100:VAL:HG13	2:R:102:PHE:H	1.83	0.42
2:V:162:ASN:ND2	2:V:202:ILE:H	2.18	0.42
1:G:19:VAL:HG13	1:G:75:ILE:HB	2.01	0.42
2:X:24:ALA:HB2	2:X:29:ILE:HG23	2.01	0.42
2:B:157:VAL:HG12	2:B:185:LEU:HD21	2.01	0.42
2:F:83:MET:HE1	2:F:94:TYR:CZ	2.55	0.42
1:M:45:LYS:NZ	3:M:222:HOH:O	2.52	0.42
1:O:159:SER:HA	1:O:178:THR:O	2.20	0.42
2:R:52:THR:HB	2:R:57:TYR:H	1.83	0.42
1:C:83:PHE:HZ	1:C:165:GLU:HG2	1.84	0.42
2:D:100:VAL:HG13	2:D:102:PHE:H	1.85	0.42
2:D:4:LEU:O	2:D:111:GLY:HA2	2.20	0.42
2:H:154:PRO:O	2:H:207:HIS:CE1	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:140:TYR:CG	1:O:141:PRO:HA	2.54	0.42
1:A:123:GLU:HA	1:A:126:LYS:HZ1	1.83	0.42
2:K:195:SER:O	2:K:199:GLN:HB2	2.20	0.42
2:R:33:TRP:HA	2:R:51:ILE:O	2.19	0.42
2:B:154:PRO:O	2:B:207:HIS:CE1	2.60	0.42
1:M:83:PHE:HB3	1:M:106:ILE:HD13	2.01	0.42
1:M:118:PHE:HA	1:M:119:PRO:HD3	1.77	0.42
1:M:167:ASP:OD2	1:M:168:SER:N	2.53	0.42
1:S:124:GLN:HE22	1:S:131:SER:HB2	1.84	0.42
2:T:91:THR:HG23	2:T:117:THR:HA	2.01	0.42
1:W:140:TYR:CD2	1:W:141:PRO:HA	2.55	0.42
1:E:145:LYS:O	1:E:196:VAL:HA	2.20	0.41
2:V:36:TRP:HD1	2:V:70:ILE:HD12	1.85	0.41
1:A:113:PRO:HB3	1:A:139:PHE:CD1	2.55	0.41
1:C:29:VAL:HG11	1:C:90:GLN:HG3	2.00	0.41
1:M:164:THR:HG22	1:M:174:SER:H	1.85	0.41
2:N:221:LYS:C	2:N:223:CYS:H	2.23	0.41
1:Q:187:GLU:HA	1:Q:211:ARG:NH2	2.36	0.41
1:Q:124:GLN:HG3	2:R:129:PHE:CE2	2.55	0.41
1:Q:145:LYS:HB2	1:Q:197:THR:HB	2.02	0.41
2:T:213:LYS:HG2	3:T:242:HOH:O	2.19	0.41
1:U:142:ARG:NH2	1:U:163:VAL:HG21	2.36	0.41
2:N:202:ILE:HA	2:N:216:LYS:O	2.20	0.41
2:T:100:VAL:O	2:T:105:TYR:HA	2.21	0.41
1:U:148:TRP:CD1	1:U:179:LEU:HD13	2.55	0.41
1:A:24:ARG:HA	1:A:69:THR:O	2.21	0.41
2:B:133:PRO:HD3	2:B:145:LEU:HB3	2.02	0.41
2:I:58:THR:CG2	2:I:60:TYR:CE1	3.03	0.41
1:J:35:TRP:CZ3	1:J:88:CYS:HB3	2.55	0.41
2:N:64:VAL:HG13	2:N:68:PHE:HB2	2.01	0.41
1:O:7:SER:HA	1:O:8:PRO:HA	1.86	0.41
2:P:52:THR:HG23	2:P:53:PRO:HD2	2.01	0.41
1:S:134:CYS:HB2	1:S:148:TRP:CZ2	2.55	0.41
2:T:35:HIS:CD2	2:T:47:TRP:HE1	2.38	0.41
2:T:83:MET:HE2	2:T:86:LEU:HD21	2.01	0.41
1:W:141:PRO:O	1:W:198:HIS:HE1	2.03	0.41
1:L:24:ARG:HA	1:L:69:THR:O	2.20	0.41
2:R:9:GLY:H	2:R:114:THR:HG21	1.85	0.41
2:X:29:ILE:HG22	2:X:34:ILE:HD11	2.02	0.41
1:E:140:TYR:CG	1:E:141:PRO:HA	2.55	0.41
2:K:200:THR:HB	2:K:217:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:83:MET:HE2	2:I:86:LEU:HD21	2.02	0.41
1:L:54:LEU:HD21	1:L:58:VAL:O	2.21	0.41
1:A:83:PHE:HD1	1:A:166:GLN:OE1	2.03	0.41
1:E:189:HIS:O	1:E:211:ARG:NH1	2.54	0.41
1:E:24:ARG:HA	1:E:69:THR:O	2.21	0.41
2:K:33:TRP:HB2	2:K:99:PHE:O	2.21	0.41
2:R:4:LEU:HG	2:R:22:CYS:SG	2.61	0.41
2:F:29:ILE:N	2:F:29:ILE:HD12	2.36	0.41
2:P:219:GLU:HB2	2:P:220:PRO:CD	2.51	0.41
2:T:154:PRO:HD2	2:T:209:PRO:CB	2.50	0.41
2:T:29:ILE:H	2:T:77:ASN:HD21	1.69	0.41
1:A:169:LYS:HE2	1:A:170:ASP:HB3	2.02	0.40
1:E:183:LYS:O	1:E:187:GLU:HG2	2.21	0.40
2:F:68:PHE:HA	2:F:82:GLN:O	2.21	0.40
1:O:187:GLU:HA	1:O:211:ARG:NH2	2.36	0.40
2:D:126:PRO:HB3	2:D:152:TYR:HB3	2.03	0.40
1:G:89:GLN:HG3	1:G:98:PHE:CE2	2.56	0.40
1:J:7:SER:HA	1:J:8:PRO:HA	1.90	0.40
1:M:166:GLN:HG3	1:M:173:TYR:CZ	2.56	0.40
2:R:37:VAL:HG22	2:R:47:TRP:HA	2.02	0.40
2:R:33:TRP:CD1	2:R:53:PRO:HD3	2.57	0.40
2:T:123:THR:HG21	2:T:209:PRO:O	2.21	0.40
2:V:162:ASN:HD21	2:V:201:TYR:HA	1.87	0.40
2:H:2:VAL:HG13	2:H:27:PHE:HD1	1.86	0.40
2:P:221:LYS:O	2:P:222:SER:C	2.59	0.40
1:Q:89:GLN:HB3	1:Q:89:GLN:HE21	1.57	0.40
2:R:52:THR:HG23	2:R:53:PRO:HD2	2.02	0.40
1:W:118:PHE:HA	1:W:119:PRO:HD3	1.77	0.40
1:G:115:VAL:HA	1:G:135:LEU:O	2.21	0.40
2:I:4:LEU:O	2:I:111:GLY:HA2	2.22	0.40
2:K:83:MET:HB3	2:K:86:LEU:HD21	2.03	0.40
1:E:161:GLU:HA	1:E:176:SER:O	2.21	0.40
2:I:64:VAL:HG13	2:I:68:PHE:HB2	2.04	0.40
1:L:7:SER:HA	1:L:8:PRO:HA	1.83	0.40
2:N:125:GLY:HA2	2:N:207:HIS:HD2	1.87	0.40
1:U:142:ARG:HG2	1:U:142:ARG:HH11	1.85	0.40
1:U:38:GLN:HA	3:U:224:HOH:O	2.20	0.40
2:V:134:SER:O	2:V:135:SER:CB	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
1	C	209/214 (98%)	203 (97%)	4 (2%)	2 (1%)	15	23
1	E	209/214 (98%)	199 (95%)	10 (5%)	0	100	100
1	G	209/214 (98%)	205 (98%)	4 (2%)	0	100	100
1	J	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
1	L	209/214 (98%)	199 (95%)	9 (4%)	1 (0%)	29	43
1	M	209/214 (98%)	197 (94%)	9 (4%)	3 (1%)	11	16
1	O	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
1	Q	209/214 (98%)	199 (95%)	8 (4%)	2 (1%)	15	23
1	S	209/214 (98%)	201 (96%)	6 (3%)	2 (1%)	15	23
1	U	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
1	W	209/214 (98%)	197 (94%)	11 (5%)	1 (0%)	29	43
2	B	214/227 (94%)	206 (96%)	8 (4%)	0	100	100
2	D	214/227 (94%)	203 (95%)	10 (5%)	1 (0%)	29	43
2	F	214/227 (94%)	203 (95%)	9 (4%)	2 (1%)	17	26
2	H	214/227 (94%)	204 (95%)	10 (5%)	0	100	100
2	I	214/227 (94%)	205 (96%)	9 (4%)	0	100	100
2	K	214/227 (94%)	206 (96%)	8 (4%)	0	100	100
2	N	214/227 (94%)	201 (94%)	13 (6%)	0	100	100
2	P	214/227 (94%)	204 (95%)	8 (4%)	2 (1%)	17	26
2	R	214/227 (94%)	203 (95%)	9 (4%)	2 (1%)	17	26
2	T	214/227 (94%)	204 (95%)	8 (4%)	2 (1%)	17	26
2	V	214/227 (94%)	207 (97%)	7 (3%)	0	100	100
2	X	214/227 (94%)	206 (96%)	8 (4%)	0	100	100
All	All	5076/5292 (96%)	4859 (96%)	197 (4%)	20 (0%)	34	48

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	109	THR
2	P	222	SER
2	F	221	LYS
1	M	183	LYS
1	Q	138	ASN
2	R	221	LYS
2	R	222	SER
1	M	138	ASN
1	M	171	SER
1	S	138	ASN
2	T	221	LYS
2	D	221	LYS
1	S	166	GLN
1	C	138	ASN
2	P	41	PRO
1	Q	204	PRO
2	T	85	SER
1	W	138	ASN
1	L	40	PRO
2	F	41	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	186/188 (99%)	145 (78%)	41 (22%)	1	0
1	C	186/188 (99%)	148 (80%)	38 (20%)	1	1
1	E	186/188 (99%)	155 (83%)	31 (17%)	2	2
1	G	186/188 (99%)	160 (86%)	26 (14%)	3	4
1	J	186/188 (99%)	153 (82%)	33 (18%)	2	1
1	L	186/188 (99%)	155 (83%)	31 (17%)	2	2
1	M	186/188 (99%)	147 (79%)	39 (21%)	1	1
1	O	186/188 (99%)	151 (81%)	35 (19%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	186/188 (99%)	150 (81%)	36 (19%)	1	1
1	S	186/188 (99%)	148 (80%)	38 (20%)	1	1
1	U	186/188 (99%)	144 (77%)	42 (23%)	1	0
1	W	186/188 (99%)	141 (76%)	45 (24%)	0	0
2	B	179/187 (96%)	138 (77%)	41 (23%)	1	0
2	D	179/187 (96%)	153 (86%)	26 (14%)	3	3
2	F	179/187 (96%)	147 (82%)	32 (18%)	2	1
2	H	179/187 (96%)	147 (82%)	32 (18%)	2	1
2	I	179/187 (96%)	150 (84%)	29 (16%)	2	2
2	K	179/187 (96%)	151 (84%)	28 (16%)	2	2
2	N	179/187 (96%)	145 (81%)	34 (19%)	1	1
2	P	179/187 (96%)	154 (86%)	25 (14%)	3	4
2	R	179/187 (96%)	144 (80%)	35 (20%)	1	1
2	T	179/187 (96%)	141 (79%)	38 (21%)	1	1
2	V	179/187 (96%)	150 (84%)	29 (16%)	2	2
2	X	179/187 (96%)	147 (82%)	32 (18%)	2	1
All	All	4380/4500 (97%)	3564 (81%)	816 (19%)	1	1

All (816) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	7	SER
1	L	9	SER
1	L	45	LYS
1	L	48	ILE
1	L	65	SER
1	L	73	LEU
1	L	83	PHE
1	L	89	GLN
1	L	90	GLN
1	L	93	THR
1	L	105	GLU
1	L	108	ARG
1	L	114	SER
1	L	122	ASP

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Mol	Chain	Res	Type
1	L	125	LEU
1	L	126	LYS
1	L	129	THR
1	L	135	LEU
1	L	147	GLN
1	L	154	LEU
1	L	158	ASN
1	L	164	THR
1	L	165	GLU
1	L	168	SER
1	L	169	LYS
1	L	171	SER
1	L	180	THR
1	L	183	LYS
1	L	201	LEU
1	L	211	ARG
2	H	1	GLU
2	H	4	LEU
2	H	11	LEU
2	H	12	VAL
2	H	13	GLN
2	H	17	SER
2	H	43	LYS
2	H	52	THR
2	H	57	TYR
2	H	58	THR
2	H	76	LYS
2	H	87	ARG
2	H	100	VAL
2	H	112	GLN
2	H	114	THR
2	H	115	LEU
2	H	117	THR
2	H	135	SER
2	H	142	THR
2	H	176	VAL
2	H	177	LEU
2	H	182	LEU
2	H	188	VAL
2	H	190	THR
2	H	194	SER
2	H	196	LEU

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Mol	Chain	Res	Type
2	H	198	THR
2	H	199	GLN
2	H	200	THR
2	H	208	LYS
2	H	216	LYS
2	H	221	LYS
1	A	3	GLN
1	A	6	GLN
1	A	9	SER
1	A	10	SER
1	A	14	SER
1	A	18	ARG
1	A	22	THR
1	A	24	ARG
1	A	30	SER
1	A	42	LYS
1	A	45	LYS
1	A	48	ILE
1	A	56	SER
1	A	73	LEU
1	A	74	THR
1	A	77	SER
1	A	83	PHE
1	A	89	GLN
1	A	105	GLU
1	A	107	LYS
1	A	108	ARG
1	A	125	LEU
1	A	135	LEU
1	A	143	GLU
1	A	147	GLN
1	A	151	ASP
1	A	164	THR
1	A	171	SER
1	A	177	SER
1	A	180	THR
1	A	181	LEU
1	A	183	LYS
1	A	188	LYS
1	A	190	LYS
1	A	194	CYS
1	A	195	GLU

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Mol	Chain	Res	Type
1	A	197	THR
1	A	201	LEU
1	A	203	SER
1	A	206	THR
1	A	210	ASN
2	B	4	LEU
2	B	11	LEU
2	B	17	SER
2	B	19	ARG
2	B	20	LEU
2	B	48	VAL
2	B	51	ILE
2	B	57	TYR
2	B	58	THR
2	B	64	VAL
2	B	65	LYS
2	B	74	THR
2	B	75	SER
2	B	100	VAL
2	B	112	GLN
2	B	114	THR
2	B	115	LEU
2	B	117	THR
2	B	127	SER
2	B	135	SER
2	B	142	THR
2	B	147	CYS
2	B	150	LYS
2	B	157	VAL
2	B	158	THR
2	B	163	SER
2	B	168	SER
2	B	177	LEU
2	B	182	LEU
2	B	184	SER
2	B	188	VAL
2	B	190	THR
2	B	193	SER
2	B	194	SER
2	B	199	GLN
2	B	200	THR
2	B	204	ASN

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Mol	Chain	Res	Type
2	B	216	LYS
2	B	217	LYS
2	B	221	LYS
2	B	223	CYS
1	C	3	GLN
1	C	9	SER
1	C	10	SER
1	C	14	SER
1	C	24	ARG
1	C	27	GLN
1	C	42	LYS
1	C	45	LYS
1	C	48	ILE
1	C	73	LEU
1	C	77	SER
1	C	79	GLN
1	C	83	PHE
1	C	90	GLN
1	C	93	THR
1	C	94	THR
1	C	105	GLU
1	C	107	LYS
1	C	108	ARG
1	C	110	VAL
1	C	114	SER
1	C	126	LYS
1	C	135	LEU
1	C	142	ARG
1	C	143	GLU
1	C	147	GLN
1	C	154	LEU
1	C	164	THR
1	C	169	LYS
1	C	188	LYS
1	C	190	LYS
1	C	195	GLU
1	C	199	GLN
1	C	201	LEU
1	C	206	THR
1	C	207	LYS
1	C	210	ASN
1	C	211	ARG

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Mol	Chain	Res	Type
2	D	1	GLU
2	D	4	LEU
2	D	11	LEU
2	D	29	ILE
2	D	57	TYR
2	D	64	VAL
2	D	85	SER
2	D	100	VAL
2	D	112	GLN
2	D	114	THR
2	D	115	LEU
2	D	117	THR
2	D	122	SER
2	D	127	SER
2	D	134	SER
2	D	135	SER
2	D	142	THR
2	D	145	LEU
2	D	158	THR
2	D	176	VAL
2	D	177	LEU
2	D	182	LEU
2	D	184	SER
2	D	190	THR
2	D	199	GLN
2	D	222	SER
1	E	1	ASP
1	E	3	GLN
1	E	14	SER
1	E	24	ARG
1	E	39	LYS
1	E	42	LYS
1	E	48	ILE
1	E	65	SER
1	E	73	LEU
1	E	83	PHE
1	E	89	GLN
1	E	90	GLN
1	E	93	THR
1	E	94	THR
1	E	105	GLU
1	E	108	ARG

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Mol	Chain	Res	Type
1	E	114	SER
1	E	125	LEU
1	E	135	LEU
1	E	143	GLU
1	E	145	LYS
1	E	154	LEU
1	E	164	THR
1	E	165	GLU
1	E	170	ASP
1	E	181	LEU
1	E	188	LYS
1	E	195	GLU
1	E	201	LEU
1	E	203	SER
1	E	207	LYS
2	F	4	LEU
2	F	11	LEU
2	F	12	VAL
2	F	20	LEU
2	F	29	ILE
2	F	46	GLU
2	F	51	ILE
2	F	52	THR
2	F	57	TYR
2	F	58	THR
2	F	76	LYS
2	F	100	VAL
2	F	103	LEU
2	F	112	GLN
2	F	114	THR
2	F	115	LEU
2	F	117	THR
2	F	127	SER
2	F	142	THR
2	F	162	ASN
2	F	168	SER
2	F	177	LEU
2	F	182	LEU
2	F	188	VAL
2	F	191	VAL
2	F	196	LEU
2	F	198	THR

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Mol	Chain	Res	Type
2	F	199	GLN
2	F	208	LYS
2	F	213	LYS
2	F	216	LYS
2	F	223	CYS
1	G	1	ASP
1	G	3	GLN
1	G	7	SER
1	G	9	SER
1	G	19	VAL
1	G	24	ARG
1	G	28	ASP
1	G	39	LYS
1	G	42	LYS
1	G	56	SER
1	G	73	LEU
1	G	89	GLN
1	G	90	GLN
1	G	107	LYS
1	G	108	ARG
1	G	125	LEU
1	G	135	LEU
1	G	143	GLU
1	G	154	LEU
1	G	164	THR
1	G	165	GLU
1	G	187	GLU
1	G	190	LYS
1	G	194	CYS
1	G	201	LEU
1	G	203	SER
2	I	1	GLU
2	I	11	LEU
2	I	20	LEU
2	I	25	SER
2	I	48	VAL
2	I	57	TYR
2	I	58	THR
2	I	62	ASP
2	I	64	VAL
2	I	65	LYS
2	I	87	ARG

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Mol	Chain	Res	Type
2	I	100	VAL
2	I	103	LEU
2	I	112	GLN
2	I	114	THR
2	I	117	THR
2	I	127	SER
2	I	142	THR
2	I	157	VAL
2	I	168	SER
2	I	177	LEU
2	I	179	SER
2	I	182	LEU
2	I	186	SER
2	I	204	ASN
2	I	206	ASN
2	I	217	LYS
2	I	221	LYS
2	I	222	SER
1	J	1	ASP
1	J	3	GLN
1	J	9	SER
1	J	18	ARG
1	J	42	LYS
1	J	45	LYS
1	J	56	SER
1	J	73	LEU
1	J	90	GLN
1	J	91	SER
1	J	93	THR
1	J	94	THR
1	J	108	ARG
1	J	114	SER
1	J	121	SER
1	J	125	LEU
1	J	129	THR
1	J	135	LEU
1	J	143	GLU
1	J	145	LYS
1	J	154	LEU
1	J	159	SER
1	J	160	GLN
1	J	164	THR

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Mol	Chain	Res	Type
1	J	169	LYS
1	J	181	LEU
1	J	183	LYS
1	J	185	ASP
1	J	188	LYS
1	J	197	THR
1	J	201	LEU
1	J	203	SER
1	J	207	LYS
2	K	1	GLU
2	K	11	LEU
2	K	12	VAL
2	K	17	SER
2	K	25	SER
2	K	52	THR
2	K	57	TYR
2	K	58	THR
2	K	64	VAL
2	K	76	LYS
2	K	100	VAL
2	K	112	GLN
2	K	114	THR
2	K	115	LEU
2	K	117	THR
2	K	134	SER
2	K	135	SER
2	K	142	THR
2	K	150	LYS
2	K	177	LEU
2	K	182	LEU
2	K	184	SER
2	K	188	VAL
2	K	198	THR
2	K	199	GLN
2	K	202	ILE
2	K	216	LYS
2	K	222	SER
1	M	7	SER
1	M	10	SER
1	M	12	SER
1	M	24	ARG
1	M	48	ILE

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Mol	Chain	Res	Type
1	M	73	LEU
1	M	83	PHE
1	M	89	GLN
1	M	90	GLN
1	M	93	THR
1	M	103	LYS
1	M	105	GLU
1	M	106	ILE
1	M	107	LYS
1	M	108	ARG
1	M	117	ILE
1	M	122	ASP
1	M	124	GLN
1	M	131	SER
1	M	134	CYS
1	M	135	LEU
1	M	137	ASN
1	M	147	GLN
1	M	154	LEU
1	M	155	GLN
1	M	161	GLU
1	M	164	THR
1	M	168	SER
1	M	176	SER
1	M	181	LEU
1	M	183	LYS
1	M	188	LYS
1	M	190	LYS
1	M	195	GLU
1	M	197	THR
1	M	201	LEU
1	M	206	THR
1	M	207	LYS
1	M	210	ASN
2	N	11	LEU
2	N	12	VAL
2	N	20	LEU
2	N	25	SER
2	N	43	LYS
2	N	52	THR
2	N	57	TYR
2	N	58	THR

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Mol	Chain	Res	Type
2	N	64	VAL
2	N	65	LYS
2	N	87	ARG
2	N	89	GLU
2	N	112	GLN
2	N	114	THR
2	N	115	LEU
2	N	117	THR
2	N	119	SER
2	N	122	SER
2	N	135	SER
2	N	145	LEU
2	N	157	VAL
2	N	158	THR
2	N	166	LEU
2	N	167	THR
2	N	179	SER
2	N	182	LEU
2	N	184	SER
2	N	186	SER
2	N	202	ILE
2	N	213	LYS
2	N	216	LYS
2	N	217	LYS
2	N	219	GLU
2	N	222	SER
1	O	1	ASP
1	O	9	SER
1	O	11	LEU
1	O	28	ASP
1	O	45	LYS
1	O	48	ILE
1	O	65	SER
1	O	72	THR
1	O	73	LEU
1	O	89	GLN
1	O	90	GLN
1	O	93	THR
1	O	94	THR
1	O	103	LYS
1	O	106	ILE
1	O	108	ARG

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Mol	Chain	Res	Type
1	O	114	SER
1	O	125	LEU
1	O	129	THR
1	O	132	VAL
1	O	135	LEU
1	O	142	ARG
1	O	143	GLU
1	O	156	SER
1	O	161	GLU
1	O	164	THR
1	O	169	LYS
1	O	171	SER
1	O	183	LYS
1	O	195	GLU
1	O	197	THR
1	O	201	LEU
1	O	202	SER
1	O	210	ASN
1	O	211	ARG
2	P	4	LEU
2	P	11	LEU
2	P	19	ARG
2	P	25	SER
2	P	43	LYS
2	P	52	THR
2	P	57	TYR
2	P	58	THR
2	P	64	VAL
2	P	76	LYS
2	P	100	VAL
2	P	112	GLN
2	P	114	THR
2	P	115	LEU
2	P	134	SER
2	P	157	VAL
2	P	158	THR
2	P	179	SER
2	P	182	LEU
2	P	186	SER
2	P	194	SER
2	P	199	GLN
2	P	217	LYS

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Mol	Chain	Res	Type
2	P	221	LYS
2	P	223	CYS
1	Q	1	ASP
1	Q	3	GLN
1	Q	5	THR
1	Q	7	SER
1	Q	18	ARG
1	Q	27	GLN
1	Q	48	ILE
1	Q	60	SER
1	Q	63	SER
1	Q	72	THR
1	Q	73	LEU
1	Q	89	GLN
1	Q	90	GLN
1	Q	93	THR
1	Q	100	GLN
1	Q	105	GLU
1	Q	106	ILE
1	Q	108	ARG
1	Q	114	SER
1	Q	117	ILE
1	Q	121	SER
1	Q	125	LEU
1	Q	126	LYS
1	Q	129	THR
1	Q	135	LEU
1	Q	143	GLU
1	Q	145	LYS
1	Q	151	ASP
1	Q	154	LEU
1	Q	161	GLU
1	Q	164	THR
1	Q	169	LYS
1	Q	183	LYS
1	Q	190	LYS
1	Q	199	GLN
1	Q	205	VAL
2	R	1	GLU
2	R	4	LEU
2	R	11	LEU
2	R	12	VAL

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Mol	Chain	Res	Type
2	R	19	ARG
2	R	20	LEU
2	R	25	SER
2	R	52	THR
2	R	57	TYR
2	R	64	VAL
2	R	76	LYS
2	R	87	ARG
2	R	100	VAL
2	R	112	GLN
2	R	114	THR
2	R	115	LEU
2	R	135	SER
2	R	145	LEU
2	R	150	LYS
2	R	155	GLU
2	R	157	VAL
2	R	166	LEU
2	R	167	THR
2	R	168	SER
2	R	170	VAL
2	R	177	LEU
2	R	186	SER
2	R	188	VAL
2	R	193	SER
2	R	196	LEU
2	R	198	THR
2	R	199	GLN
2	R	206	ASN
2	R	216	LYS
2	R	222	SER
1	S	1	ASP
1	S	3	GLN
1	S	7	SER
1	S	18	ARG
1	S	19	VAL
1	S	22	THR
1	S	27	GLN
1	S	42	LYS
1	S	48	ILE
1	S	56	SER
1	S	73	LEU

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Mol	Chain	Res	Type
1	S	78	LEU
1	S	89	GLN
1	S	91	SER
1	S	93	THR
1	S	94	THR
1	S	106	ILE
1	S	107	LYS
1	S	108	ARG
1	S	114	SER
1	S	121	SER
1	S	122	ASP
1	S	125	LEU
1	S	142	ARG
1	S	143	GLU
1	S	147	GLN
1	S	154	LEU
1	S	160	GLN
1	S	161	GLU
1	S	164	THR
1	S	169	LYS
1	S	171	SER
1	S	187	GLU
1	S	195	GLU
1	S	203	SER
1	S	207	LYS
1	S	210	ASN
1	S	211	ARG
2	T	1	GLU
2	T	11	LEU
2	T	12	VAL
2	T	17	SER
2	T	19	ARG
2	T	25	SER
2	T	29	ILE
2	T	43	LYS
2	T	51	ILE
2	T	52	THR
2	T	57	TYR
2	T	58	THR
2	T	62	ASP
2	T	76	LYS
2	T	87	ARG

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Mol	Chain	Res	Type
2	T	89	GLU
2	T	100	VAL
2	T	112	GLN
2	T	114	THR
2	T	115	LEU
2	T	117	THR
2	T	124	LYS
2	T	134	SER
2	T	135	SER
2	T	157	VAL
2	T	158	THR
2	T	167	THR
2	T	168	SER
2	T	177	LEU
2	T	182	LEU
2	T	194	SER
2	T	199	GLN
2	T	204	ASN
2	T	208	LYS
2	T	213	LYS
2	T	216	LYS
2	T	217	LYS
2	T	221	LYS
1	U	1	ASP
1	U	5	THR
1	U	7	SER
1	U	9	SER
1	U	14	SER
1	U	20	THR
1	U	24	ARG
1	U	52	SER
1	U	56	SER
1	U	73	LEU
1	U	89	GLN
1	U	90	GLN
1	U	91	SER
1	U	93	THR
1	U	107	LYS
1	U	108	ARG
1	U	109	THR
1	U	114	SER
1	U	125	LEU

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Mol	Chain	Res	Type
1	U	131	SER
1	U	135	LEU
1	U	142	ARG
1	U	143	GLU
1	U	145	LYS
1	U	152	ASN
1	U	158	ASN
1	U	160	GLN
1	U	163	VAL
1	U	164	THR
1	U	168	SER
1	U	169	LYS
1	U	171	SER
1	U	181	LEU
1	U	185	ASP
1	U	187	GLU
1	U	188	LYS
1	U	194	CYS
1	U	197	THR
1	U	201	LEU
1	U	203	SER
1	U	207	LYS
1	U	210	ASN
2	V	1	GLU
2	V	3	GLN
2	V	11	LEU
2	V	12	VAL
2	V	20	LEU
2	V	51	ILE
2	V	52	THR
2	V	57	TYR
2	V	58	THR
2	V	87	ARG
2	V	100	VAL
2	V	112	GLN
2	V	114	THR
2	V	115	LEU
2	V	117	THR
2	V	124	LYS
2	V	135	SER
2	V	142	THR
2	V	157	VAL

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Mol	Chain	Res	Type
2	V	158	THR
2	V	177	LEU
2	V	188	VAL
2	V	193	SER
2	V	198	THR
2	V	199	GLN
2	V	204	ASN
2	V	213	LYS
2	V	216	LYS
2	V	221	LYS
1	W	1	ASP
1	W	5	THR
1	W	6	GLN
1	W	7	SER
1	W	11	LEU
1	W	18	ARG
1	W	31	THR
1	W	42	LYS
1	W	45	LYS
1	W	48	ILE
1	W	56	SER
1	W	73	LEU
1	W	83	PHE
1	W	90	GLN
1	W	91	SER
1	W	93	THR
1	W	94	THR
1	W	105	GLU
1	W	106	ILE
1	W	107	LYS
1	W	108	ARG
1	W	126	LYS
1	W	131	SER
1	W	135	LEU
1	W	143	GLU
1	W	145	LYS
1	W	147	GLN
1	W	149	LYS
1	W	151	ASP
1	W	164	THR
1	W	165	GLU
1	W	168	SER

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Mol	Chain	Res	Type
1	W	169	LYS
1	W	171	SER
1	W	172	THR
1	W	180	THR
1	W	181	LEU
1	W	183	LYS
1	W	189	HIS
1	W	190	LYS
1	W	194	CYS
1	W	197	THR
1	W	201	LEU
1	W	206	THR
1	W	207	LYS
2	X	1	GLU
2	X	4	LEU
2	X	11	LEU
2	X	20	LEU
2	X	29	ILE
2	X	52	THR
2	X	57	TYR
2	X	58	THR
2	X	77	ASN
2	X	87	ARG
2	X	100	VAL
2	X	103	LEU
2	X	112	GLN
2	X	114	THR
2	X	115	LEU
2	X	117	THR
2	X	120	SER
2	X	142	THR
2	X	150	LYS
2	X	168	SER
2	X	177	LEU
2	X	184	SER
2	X	185	LEU
2	X	186	SER
2	X	188	VAL
2	X	193	SER
2	X	194	SER
2	X	199	GLN
2	X	208	LYS

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Mol	Chain	Res	Type
2	X	216	LYS
2	X	221	LYS
2	X	222	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	79	GLN
1	L	89	GLN
1	L	152	ASN
1	L	158	ASN
1	L	160	GLN
1	L	198	HIS
2	H	13	GLN
2	H	35	HIS
2	H	77	ASN
2	H	207	HIS
1	A	37	GLN
1	A	89	GLN
1	A	198	HIS
2	B	162	ASN
2	B	207	HIS
1	C	37	GLN
1	C	89	GLN
1	C	147	GLN
1	C	160	GLN
1	C	198	HIS
2	D	207	HIS
1	E	89	GLN
1	E	160	GLN
1	E	198	HIS
1	E	210	ASN
2	F	3	GLN
2	F	207	HIS
1	G	3	GLN
1	G	89	GLN
1	G	152	ASN
1	G	160	GLN
1	G	198	HIS
1	G	210	ASN
2	I	35	HIS
2	I	162	ASN

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Mol	Chain	Res	Type
2	I	199	GLN
2	I	207	HIS
1	J	89	GLN
1	J	160	GLN
1	J	198	HIS
2	K	35	HIS
2	K	77	ASN
2	K	207	HIS
1	M	89	GLN
1	M	124	GLN
1	M	160	GLN
1	M	198	HIS
2	N	13	GLN
2	N	162	ASN
2	N	204	ASN
2	N	206	ASN
2	N	207	HIS
1	O	89	GLN
1	O	137	ASN
1	O	147	GLN
1	O	160	GLN
1	O	198	HIS
1	O	210	ASN
2	P	13	GLN
2	P	35	HIS
2	P	77	ASN
2	P	162	ASN
2	P	199	GLN
1	Q	89	GLN
1	Q	100	GLN
1	Q	137	ASN
1	Q	166	GLN
1	Q	198	HIS
1	Q	210	ASN
2	R	35	HIS
2	R	77	ASN
2	R	178	GLN
2	R	207	HIS
1	S	79	GLN
1	S	89	GLN
1	S	90	GLN
1	S	124	GLN

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Mol	Chain	Res	Type
1	S	137	ASN
1	S	138	ASN
1	S	147	GLN
1	S	160	GLN
1	S	198	HIS
1	S	210	ASN
2	T	77	ASN
2	T	162	ASN
2	T	207	HIS
1	U	89	GLN
1	U	124	GLN
1	U	137	ASN
1	U	152	ASN
1	U	155	GLN
1	U	158	ASN
1	U	160	GLN
1	U	198	HIS
1	U	210	ASN
2	V	35	HIS
2	V	77	ASN
2	V	162	ASN
2	V	207	HIS
1	W	198	HIS
2	X	3	GLN
2	X	35	HIS
2	X	77	ASN
2	X	162	ASN
2	X	207	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data 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	211/214 (98%)	-0.20	4 (1%) 66 63	5, 11, 14, 17	0
1	C	211/214 (98%)	-0.26	2 (0%) 84 83	5, 11, 14, 16	0
1	E	211/214 (98%)	-0.25	0 100 100	7, 11, 13, 15	0
1	G	211/214 (98%)	-0.57	0 100 100	4, 10, 14, 17	0
1	J	211/214 (98%)	-0.41	1 (0%) 91 91	6, 10, 13, 18	0
1	L	211/214 (98%)	0.07	6 (2%) 53 49	5, 11, 14, 16	0
1	M	211/214 (98%)	0.28	25 (11%) 4 3	7, 11, 13, 16	0
1	O	211/214 (98%)	-0.37	2 (0%) 84 83	6, 11, 14, 17	0
1	Q	211/214 (98%)	0.11	10 (4%) 31 28	6, 11, 13, 15	0
1	S	211/214 (98%)	0.14	8 (3%) 40 36	7, 11, 13, 15	0
1	U	211/214 (98%)	-0.18	7 (3%) 46 43	7, 11, 14, 15	0
1	W	211/214 (98%)	0.07	4 (1%) 66 63	7, 10, 13, 14	0
2	B	218/227 (96%)	-0.27	6 (2%) 53 49	6, 10, 14, 20	0
2	D	218/227 (96%)	-0.37	6 (2%) 53 49	5, 10, 14, 19	0
2	F	218/227 (96%)	-0.17	9 (4%) 37 33	6, 10, 14, 19	0
2	H	218/227 (96%)	-0.22	11 (5%) 28 25	5, 10, 14, 21	0
2	I	218/227 (96%)	-0.48	2 (0%) 84 83	6, 10, 14, 22	0
2	K	218/227 (96%)	-0.17	6 (2%) 53 49	5, 10, 15, 22	0
2	N	218/227 (96%)	-0.05	17 (7%) 13 10	4, 11, 13, 22	0
2	P	218/227 (96%)	-0.45	1 (0%) 91 91	5, 10, 14, 22	0
2	R	218/227 (96%)	-0.15	9 (4%) 37 33	6, 10, 13, 23	0
2	T	218/227 (96%)	-0.23	4 (1%) 68 65	6, 10, 14, 21	0
2	V	218/227 (96%)	-0.25	4 (1%) 68 65	3, 10, 14, 22	0
2	X	218/227 (96%)	-0.29	4 (1%) 68 65	6, 10, 13, 22	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5148/5292 (97%)	-0.20	148 (2%) 51 48	3, 10, 14, 23	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	223	CYS	8.9
2	N	198	THR	7.9
2	H	223	CYS	6.4
2	F	223	CYS	6.3
2	B	223	CYS	6.3
2	K	223	CYS	6.1
2	H	165	ALA	5.6
2	K	222	SER	5.5
2	R	222	SER	5.4
1	M	122	ASP	5.3
1	M	183	LYS	5.2
2	N	223	CYS	5.2
1	L	184	ALA	5.2
2	T	223	CYS	5.2
2	X	223	CYS	5.1
1	M	184	ALA	5.0
2	R	197	GLY	4.9
2	I	223	CYS	4.9
2	N	222	SER	4.9
2	F	222	SER	4.7
2	P	223	CYS	4.7
1	M	151	ASP	4.6
2	T	141	GLY	4.5
1	M	154	LEU	4.4
2	F	198	THR	4.3
2	V	141	GLY	4.2
1	U	184	ALA	4.2
2	N	197	GLY	4.1
1	Q	190	LYS	3.9
1	M	187	GLU	3.8
2	V	135	SER	3.8
1	M	201	LEU	3.8
1	S	154	LEU	3.7
2	H	222	SER	3.7
2	V	222	SER	3.7
1	S	184	ALA	3.7
1	L	157	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	145	LYS	3.6
2	N	1	GLU	3.6
2	N	135	SER	3.6
1	O	184	ALA	3.5
2	D	198	THR	3.4
1	L	156	SER	3.4
1	Q	157	GLY	3.4
2	B	222	SER	3.4
1	L	154	LEU	3.3
1	U	156	SER	3.3
1	S	133	VAL	3.2
2	N	201	TYR	3.2
1	M	128	GLY	3.2
2	X	198	THR	3.1
2	K	197	GLY	3.1
2	N	195	SER	3.1
2	K	198	THR	3.1
2	N	130	PRO	3.1
1	M	197	THR	3.0
1	M	83	PHE	3.0
1	S	188	LYS	3.0
2	N	141	GLY	3.0
1	M	209	PHE	2.9
2	H	198	THR	2.9
2	N	200	THR	2.9
1	Q	210	ASN	2.8
2	H	195	SER	2.7
1	W	109	THR	2.7
1	M	194	CYS	2.7
2	T	193	SER	2.7
1	S	76	SER	2.6
2	R	165	ALA	2.6
1	U	154	LEU	2.6
1	U	210	ASN	2.6
1	Q	203	SER	2.6
1	Q	205	VAL	2.5
2	R	221	LYS	2.5
1	Q	199	GLN	2.5
1	S	202	SER	2.5
2	N	199	GLN	2.5
1	Q	148	TRP	2.5
1	M	131	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	169	LYS	2.5
2	R	196	LEU	2.5
1	M	150	VAL	2.5
2	R	135	SER	2.4
1	M	157	GLY	2.4
2	K	199	GLN	2.4
1	Q	191	VAL	2.4
2	B	198	THR	2.4
1	A	168	SER	2.4
1	W	187	GLU	2.4
2	F	195	SER	2.4
1	S	111	ALA	2.4
1	U	202	SER	2.4
2	F	161	TRP	2.4
2	B	196	LEU	2.4
2	H	194	SER	2.4
1	U	157	GLY	2.4
2	F	202	ILE	2.4
2	H	217	LYS	2.3
2	B	194	SER	2.3
2	N	192	PRO	2.3
2	K	195	SER	2.3
1	M	196	VAL	2.3
2	D	222	SER	2.3
1	S	117	ILE	2.3
2	N	132	ALA	2.3
1	M	206	THR	2.3
1	J	184	ALA	2.3
2	H	202	ILE	2.3
2	R	213	LYS	2.3
1	A	210	ASN	2.3
1	M	204	PRO	2.3
2	R	134	SER	2.3
2	R	1	GLU	2.3
1	A	169	LYS	2.3
2	N	146	GLY	2.2
2	T	192	PRO	2.2
1	U	107	LYS	2.2
2	D	223	CYS	2.2
1	M	191	VAL	2.2
1	W	201	LEU	2.2
2	N	165	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	152	ASN	2.2
2	I	222	SER	2.2
2	H	166	LEU	2.2
2	H	196	LEU	2.2
1	W	188	LYS	2.1
1	M	126	LYS	2.1
2	F	164	GLY	2.1
2	D	195	SER	2.1
2	B	1	GLU	2.1
2	F	165	ALA	2.1
2	X	134	SER	2.1
1	L	152	ASN	2.1
1	C	191	VAL	2.1
2	F	162	ASN	2.1
1	Q	209	PHE	2.1
2	D	142	THR	2.0
2	H	221	LYS	2.0
2	D	197	GLY	2.0
2	X	141	GLY	2.0
1	A	83	PHE	2.0
1	M	119	PRO	2.0
1	C	190	LYS	2.0
1	M	192	TYR	2.0
1	O	126	LYS	2.0
1	Q	188	LYS	2.0
2	N	217	LYS	2.0
1	L	122	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.