



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:00 PM UTC

PDB ID : 2FJF / pdb_00002fjf
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 types of validation reports are described at

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

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

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

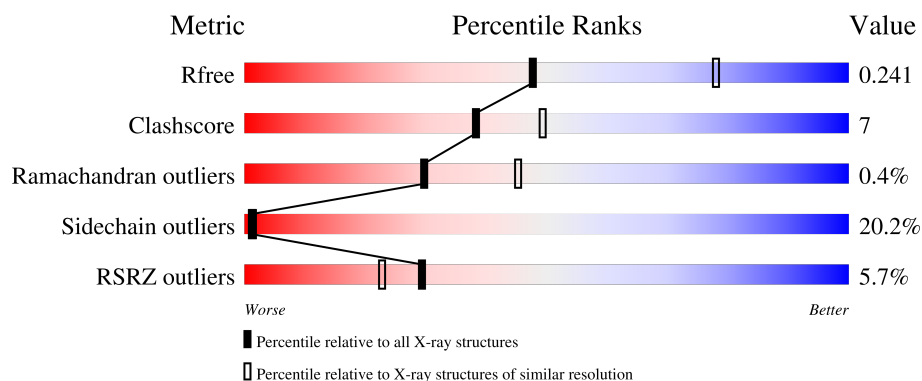
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	214	64% 28% 7% .
1	C	214	2% 77% 18% ..
1	E	214	74% 22% ..
1	G	214	74% 20% 5% .
1	J	214	6% 72% 24% ..

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Mol	Chain	Length	Quality of chain
1	L	214	
1	M	214	
1	O	214	
1	Q	214	
1	S	214	
1	U	214	
1	W	214	
2	B	227	
2	D	227	
2	F	227	
2	H	227	
2	I	227	
2	K	227	
2	N	227	
2	P	227	
2	R	227	
2	T	227	
2	V	227	
2	X	227	

2 Entry composition

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
1	L	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	A	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	C	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	E	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	G	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	J	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	M	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	O	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	Q	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	S	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	U	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	W	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			

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

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

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

- Molecule 3 is water.

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

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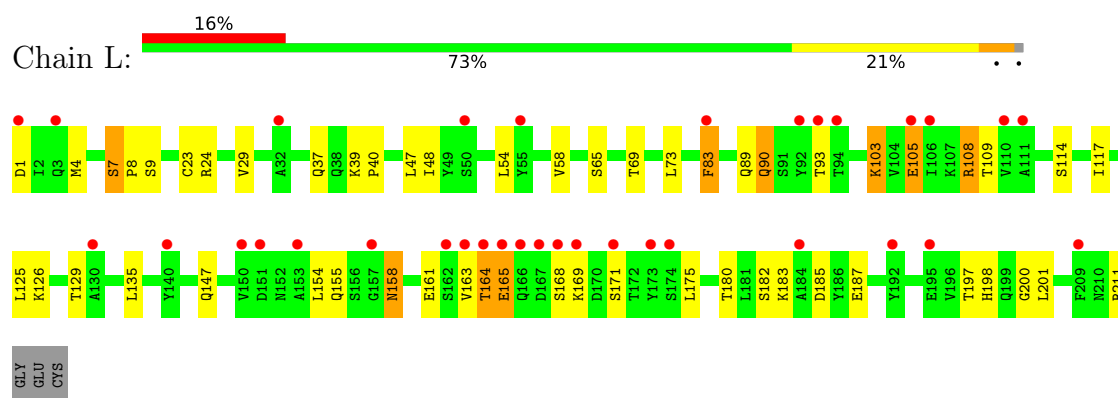
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	52	Total 52	O 52	0	0
3	J	35	Total 35	O 35	0	0
3	K	53	Total 53	O 53	0	0
3	M	17	Total 17	O 17	0	0
3	N	24	Total 24	O 24	0	0
3	O	31	Total 31	O 31	0	0
3	P	52	Total 52	O 52	0	0
3	Q	15	Total 15	O 15	0	0
3	R	21	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

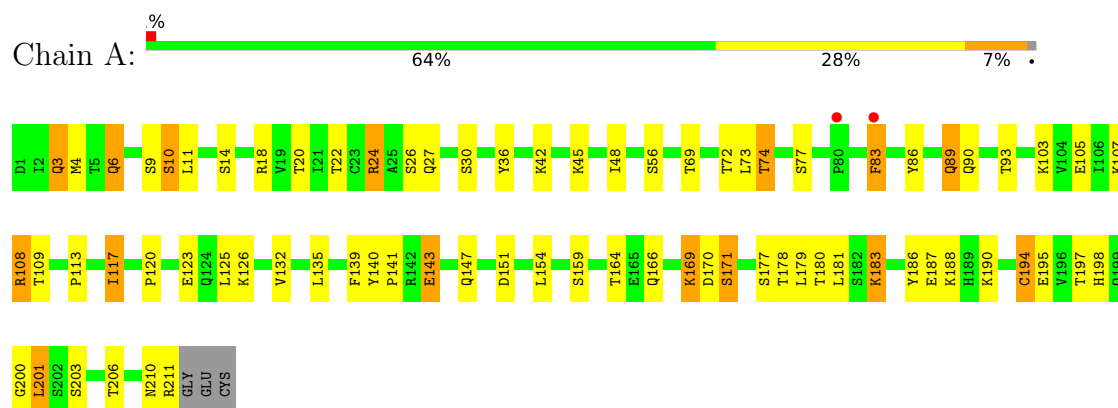
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

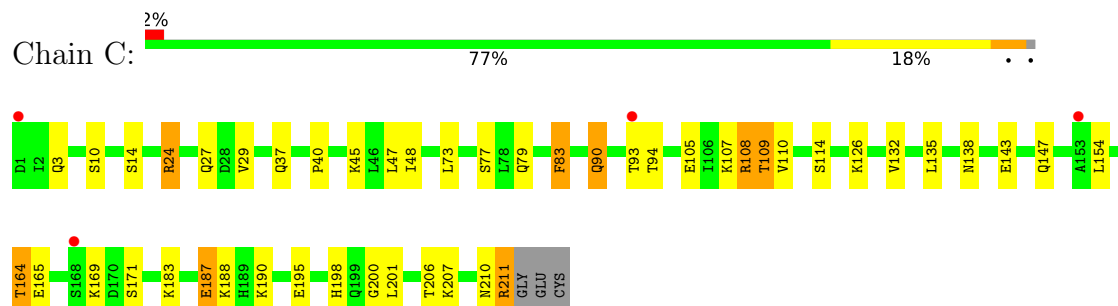
- Molecule 1: Light Chain of a VEGF binding Antibody



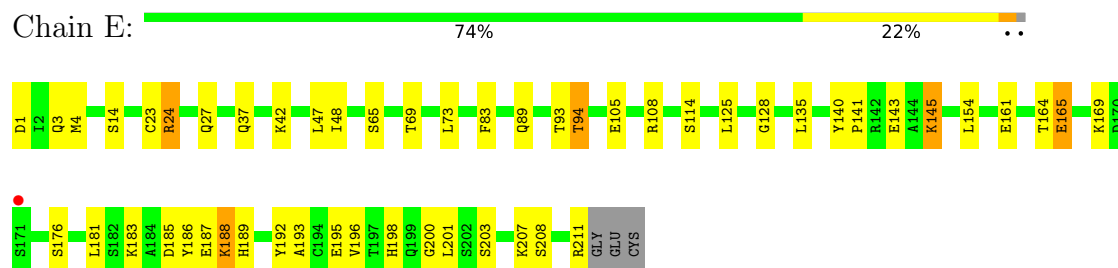
- Molecule 1: Light Chain of a VEGF binding Antibody



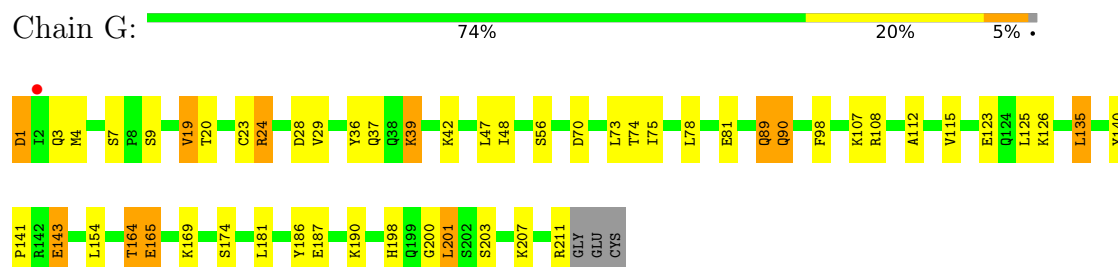
- Molecule 1: Light Chain of a VEGF binding Antibody



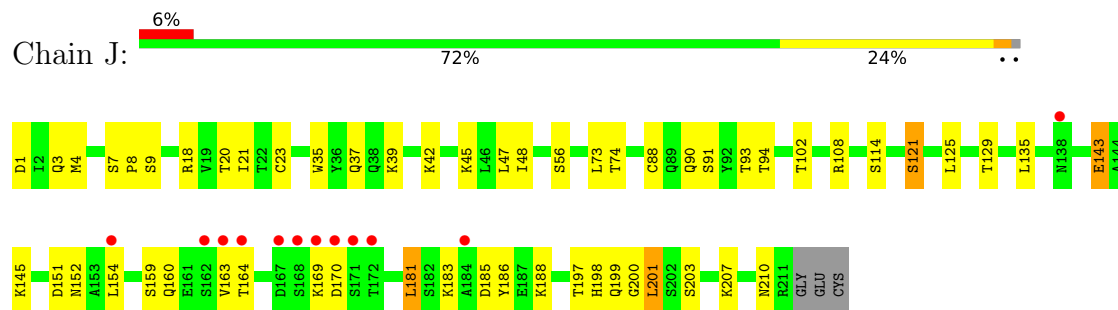
- Molecule 1: Light Chain of a VEGF binding Antibody



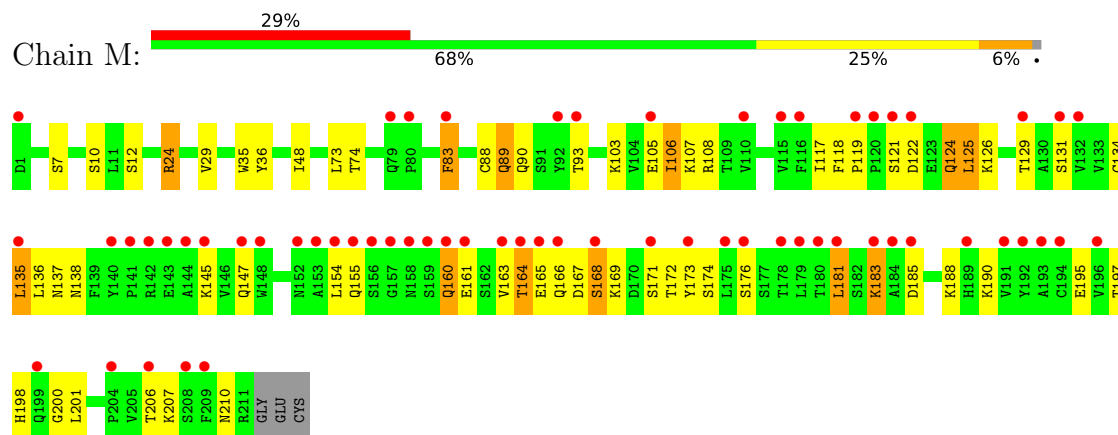
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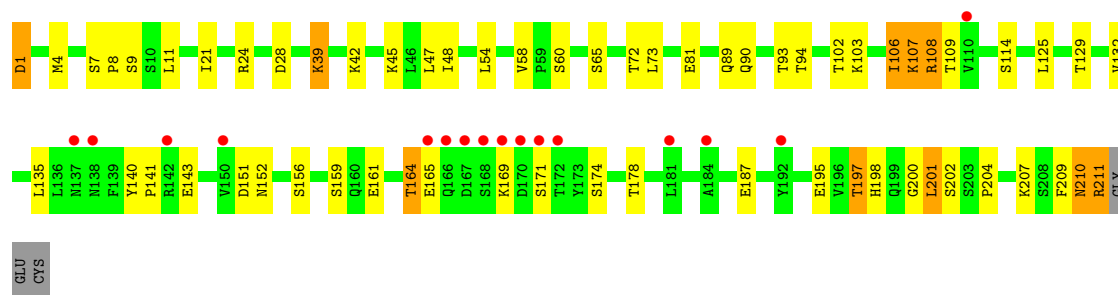


- Molecule 1: Light Chain of a VEGF binding Antibody

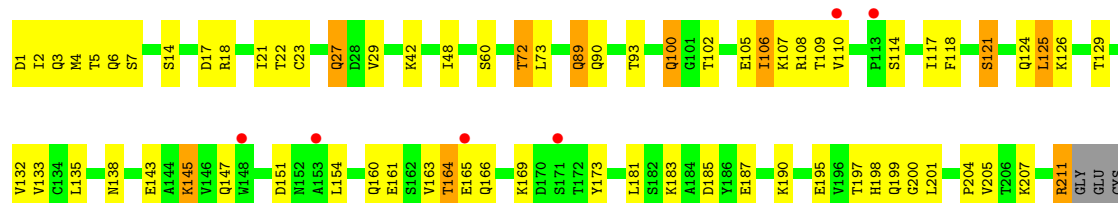


- Molecule 1: Light Chain of a VEGF binding Antibody

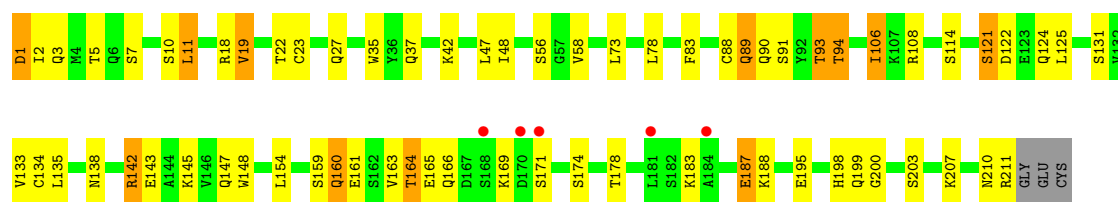




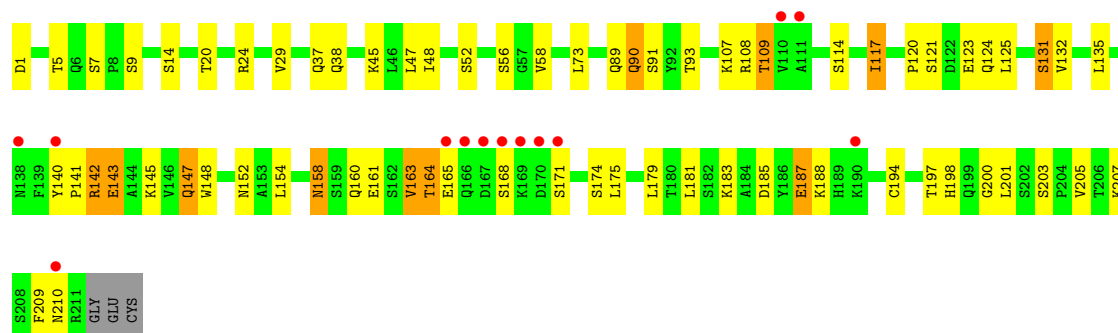
• Molecule 1: Light Chain of a VEGF binding Antibody



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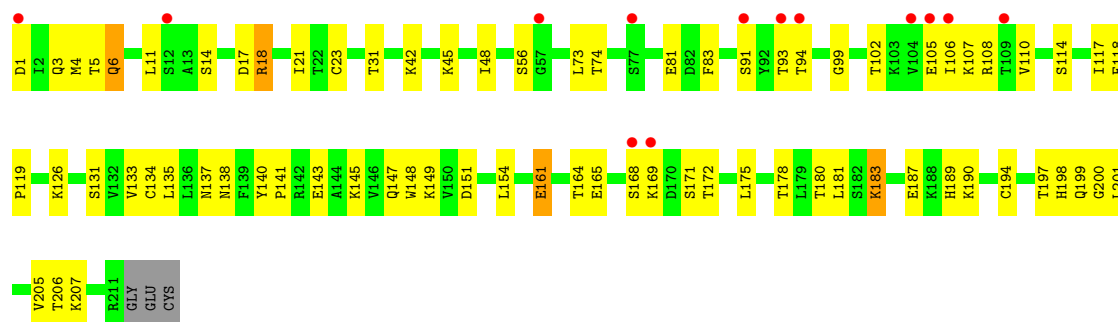


• Molecule 1: Light Chain of a VEGF binding Antibody

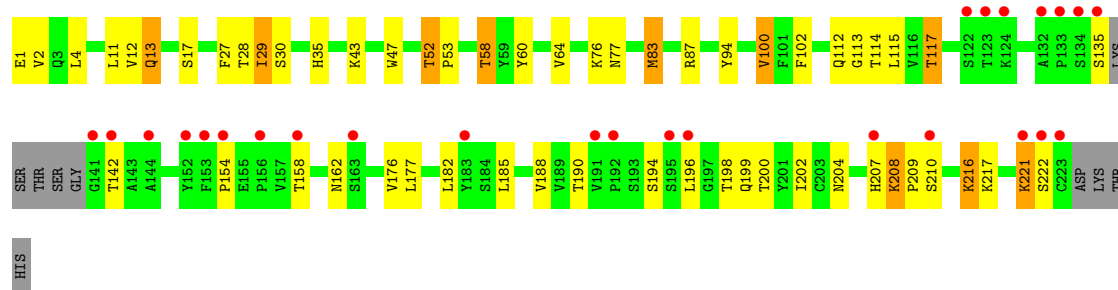


• Molecule 1: Light Chain of a VEGF binding Antibody

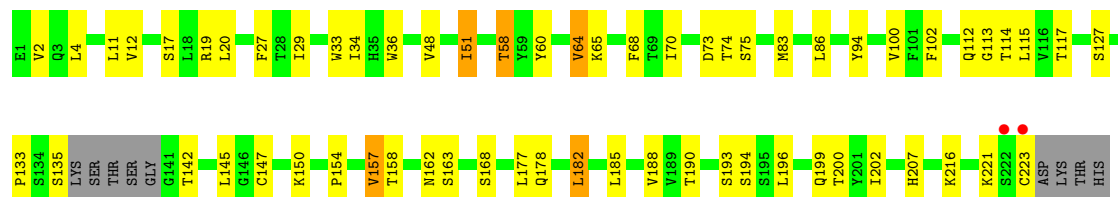




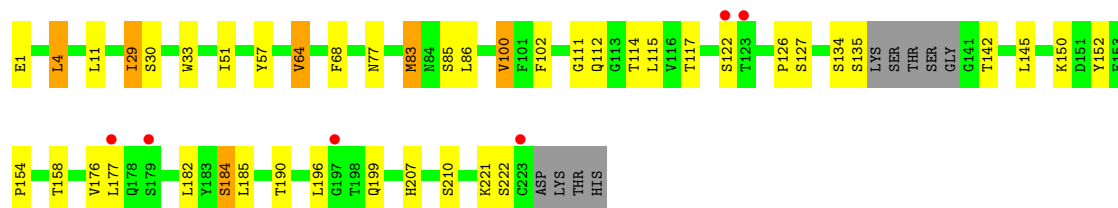
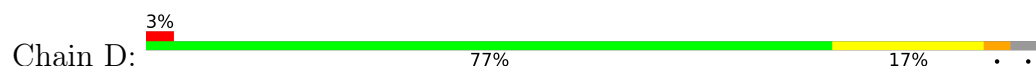
● Molecule 2: Heavy Chain of a VEGF binding Antibody



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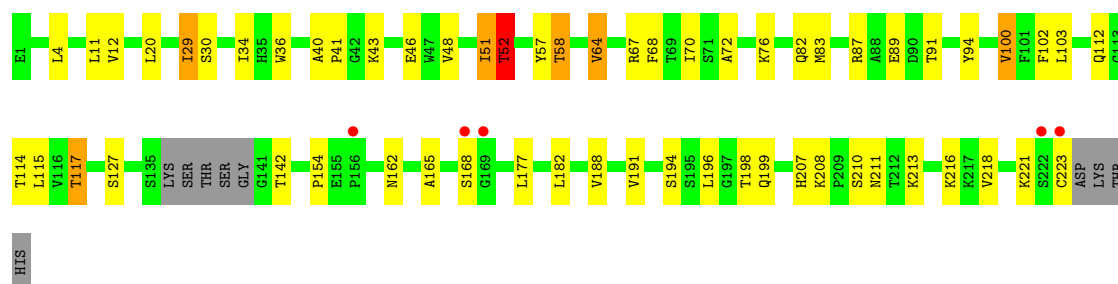


● Molecule 2: Heavy Chain of a VEGF binding Antibody

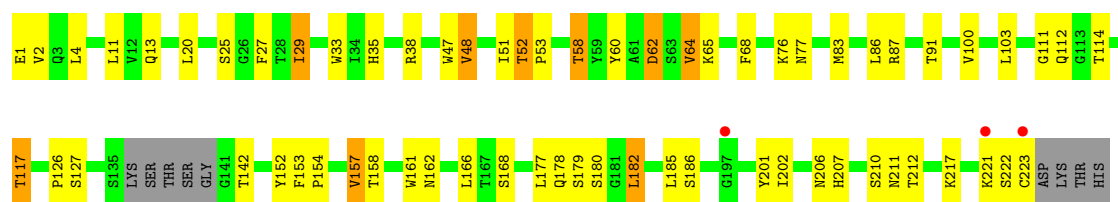


● Molecule 2: Heavy Chain of a VEGF binding Antibody

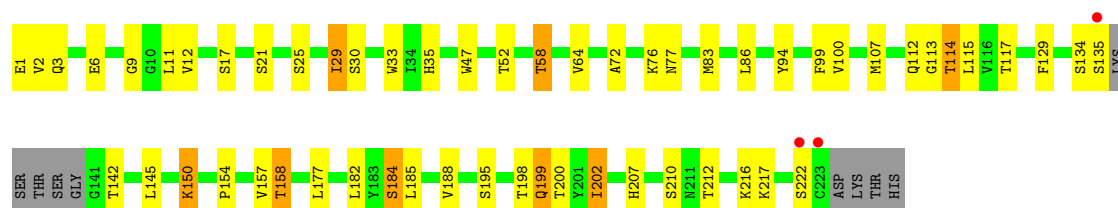




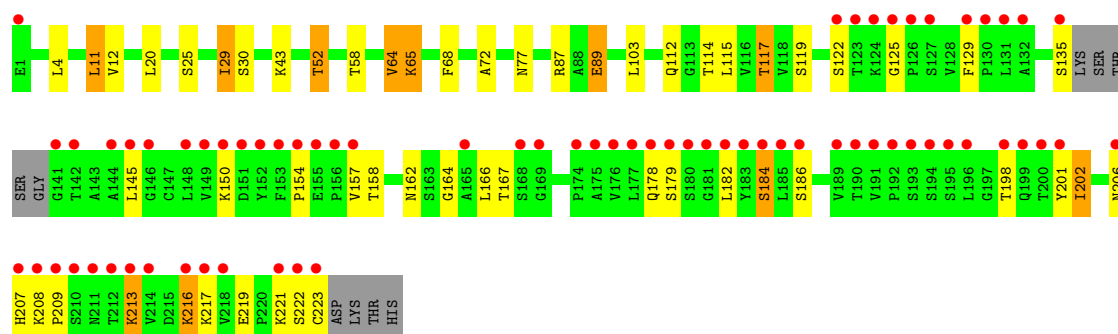
• Molecule 2: Heavy Chain of a VEGF binding Antibody



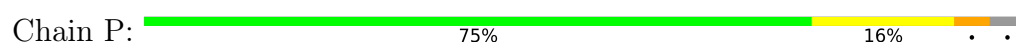
• Molecule 2: Heavy Chain of a VEGF binding Antibody

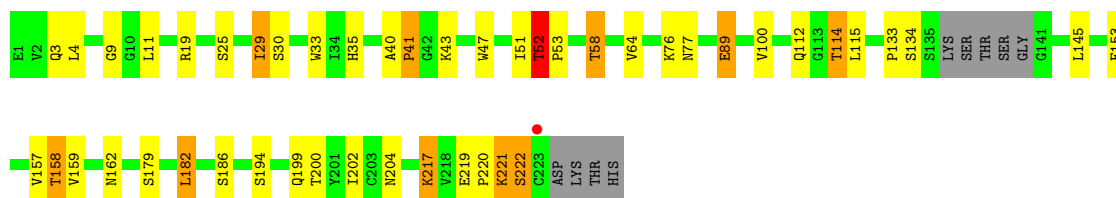


• Molecule 2: Heavy Chain of a VEGF binding Antibody

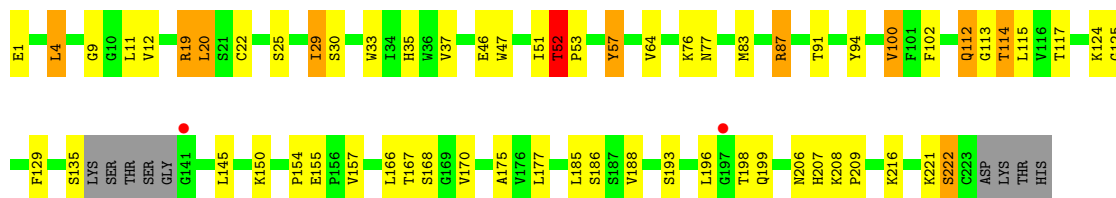


• Molecule 2: Heavy Chain of a VEGF binding Antibody

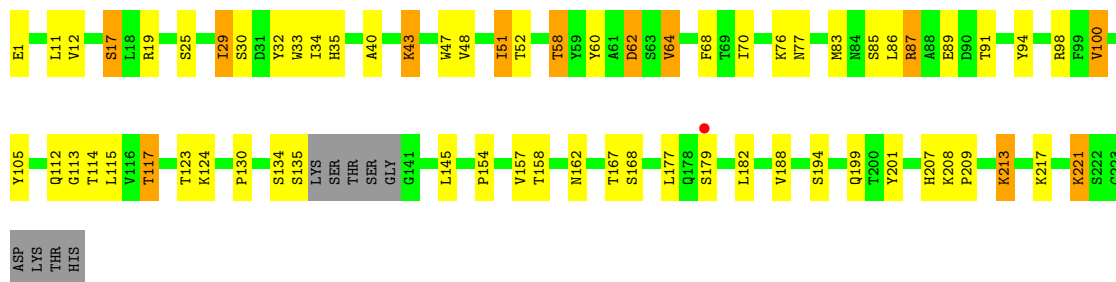




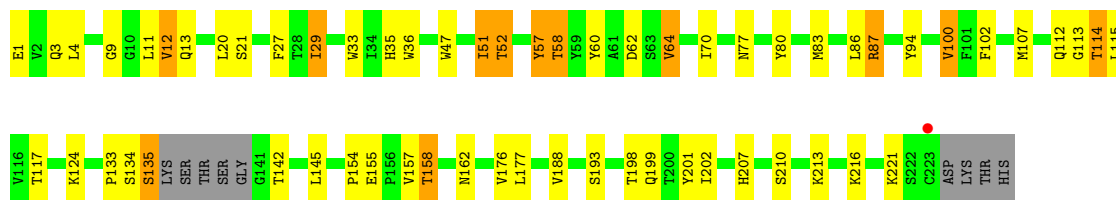
• Molecule 2: Heavy Chain of a VEGF binding Antibody



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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 20.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.65) 99.6 (20.00-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.64Å)	Xtriage
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 (2.18%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	39642	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/1653	0.84	0/2248
1	C	0.46	0/1653	0.85	0/2248
1	E	0.47	0/1653	0.85	2/2248 (0.1%)
1	G	0.53	0/1653	0.83	0/2248
1	J	0.50	0/1653	0.87	0/2248
1	L	0.49	0/1653	0.85	0/2248
1	M	0.52	0/1653	0.88	0/2248
1	O	0.49	0/1653	0.85	0/2248
1	Q	0.48	0/1653	0.85	0/2248
1	S	0.45	0/1653	0.81	0/2248
1	U	0.48	0/1653	0.83	0/2248
1	W	0.47	0/1653	0.86	0/2248
2	B	0.55	1/1677 (0.1%)	0.89	0/2290
2	D	0.52	1/1677 (0.1%)	0.86	0/2290
2	F	0.53	0/1677	0.91	1/2290 (0.0%)
2	H	0.56	1/1677 (0.1%)	0.89	0/2290
2	I	0.59	0/1677	0.88	0/2290
2	K	0.53	0/1677	0.87	2/2290 (0.1%)
2	N	0.50	0/1677	0.85	1/2290 (0.0%)
2	P	0.54	0/1677	0.88	2/2290 (0.1%)
2	R	0.50	0/1677	0.86	1/2290 (0.0%)
2	T	0.51	0/1677	0.88	0/2290
2	V	0.51	0/1677	0.88	0/2290
2	X	0.52	0/1677	0.85	1/2290 (0.0%)
All	All	0.51	3/39960 (0.0%)	0.86	10/54456 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	83	MET	SD-CE	-5.33	1.66	1.79
2	H	83	MET	SD-CE	-5.33	1.66	1.79
2	D	83	MET	SD-CE	-5.20	1.66	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	94	THR	CB-CA-C	6.49	117.66	108.76
1	E	128	GLY	N-CA-C	5.64	121.79	115.08
2	X	151	ASP	N-CA-C	5.56	117.41	110.91
2	K	3	GLN	N-CA-C	5.39	116.71	108.52
2	P	3	GLN	N-CA-C	5.33	116.39	108.60
2	F	52	THR	N-CA-CB	-5.17	103.78	110.03
2	N	52	THR	N-CA-CB	-5.09	103.83	109.74
2	R	52	THR	N-CA-CB	-5.07	102.78	109.78
2	K	2	VAL	N-CA-C	5.03	116.07	109.58
2	P	52	THR	N-CA-CB	-5.02	102.85	109.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1617	0	1573	25	0
1	C	1617	0	1573	13	0
1	E	1617	0	1573	15	0
1	G	1617	0	1573	25	0
1	J	1617	0	1573	17	0
1	L	1617	0	1573	16	0
1	M	1617	0	1573	20	0
1	O	1617	0	1573	22	0
1	Q	1617	0	1573	21	0
1	S	1617	0	1573	26	0
1	U	1617	0	1573	26	0
1	W	1617	0	1573	17	0
2	B	1633	0	1592	17	0
2	D	1633	0	1592	13	0
2	F	1633	0	1592	22	0
2	H	1633	0	1592	28	0
2	I	1633	0	1592	32	0
2	K	1633	0	1592	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1633	0	1592	29	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	35	0
2	X	1633	0	1592	23	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
3	K	53	0	0	2	0
3	L	22	0	0	0	0
3	M	17	0	0	0	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	529	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 (529) 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:HG3	2:R:19:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OD1	1:G:1:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	2:R:19:ARG:NH1	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:O:1:ASP:N	3:O:234:HOH:O	2.29	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
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
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
1:U:143:GLU:CD	1:U:143:GLU:H	2.06	0.62
2:X:154:PRO:O	2:X:207:HIS:HE1	1.83	0.62
2:I:83:MET:HE2	2:I:86:LEU:HD21	1.81	0.62
2:V:87:ARG:HH11	2:V:87:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:202:ILE:HD12	2:H:204:ASN:HD21	1.65	0.59
2:B:58:THR:HG23	2:B:60:TYR:CE1	2.38	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:L:4:MET:HE3	1:L:23:CYS:SG	2.44	0.58
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
1:J:4:MET:HE3	1:J:23:CYS:SG	2.43	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
2:H:117:THR:CG2	3:H:253:HOH:O	2.52	0.56
1:G:29:VAL:HG11	1:G:90:GLN:HG3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:83:PHE:C	1:A:83:PHE:CD2	2.83	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
1:O:209:PHE:C	1:O:210:ASN:HD22	2.14	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
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
2:P:89:GLU:CD	2:P:89:GLU:H	2.16	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
2:D:83:MET:HE2	2:D:86:LEU:HD21	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:83:PHE:CD1	1:L:83:PHE:C	2.87	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
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: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
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
1:U:143:GLU:CD	1:U:143:GLU:N	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:T:83:MET:HE2	2:T:86:LEU:HD21	1.94	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:36:TRP:HD1	2:F:70:ILE:HD12	1.77	0.49
2:F:165:ALA:O	1:W:18:ARG:NH2	2.45	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:HD22	1:U:158:ASN:H	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
2:T:87:ARG:NH1	2:T:87:ARG:HG3	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
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
1:A:143:GLU:H	1:A:143:GLU:CD	2.20	0.48
2:F:40:ALA:HB3	2:F:43:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:29:ILE:HD12	2:R:30:SER:H	1.77	0.48
2:R:87:ARG:HH11	2:R:87:ARG:CG	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:39:LYS:NZ	1:O:81:GLU:O	2.46	0.48
1:O:164:THR:CG2	1:O:174:SER:H	2.24	0.48
2:R:87:ARG:HH11	2:R:87:ARG:CB	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:I:178:GLN:C	2:I:180:SER:H	2.21	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
2:N:162:ASN:C	2:N:164:GLY:H	2.21	0.48
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.95	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
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:4:MET:SD	1:J:90:GLN:HB2	2.54	0.47
1:J:181:LEU:HD13	1:J:186:TYR:HB2	1.96	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:4:LEU:HD21	2:I:27:PHE:HZ	1.79	0.47
2:I:153:PHE:HB2	2:I:182:LEU:HD12	1.96	0.47
2:H:58:THR:HG23	2:H:60:TYR:CE1	2.50	0.47
1:C:24:ARG:O	1:C:24:ARG:HG3	2.14	0.47
2:K:157:VAL:CG1	2:K:185:LEU:HD21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:198:HIS:HD2	1:L:200:GLY:H	1.59	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: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:O:197:THR:HG23	1:O:204:PRO:HG3	1.97	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:OD2	2:T:62:ASP:N	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:N:221:LYS:C	2:N:223:CYS:H	2.23	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:64:VAL:HG13	2:D:68:PHE:HB2	1.97	0.46
2:D:102:PHE:CD2	2:K:72:ALA:HB3	2.50	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
2:I:211:ASN:CB	2:N:11:LEU:HD13	2.46	0.46
1:M:24:ARG:HE	1:M:24:ARG:HB2	1.54	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:HG3	2:T:87:ARG:HH11	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:A:123:GLU:HA	1:A:126:LYS:HZ3	1.81	0.45
1:E:185:ASP:HA	1:E:188:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:37:GLN:HB2	1:U:47:LEU:HD11	1.97	0.45
2:H:29:ILE:HD12	2:H:30:SER:N	2.32	0.45
1:C:83:PHE:CZ	1:C:165:GLU:HG3	2.51	0.45
1:O:164:THR:HG21	3:O:227:HOH:O	2.16	0.45
2:V:35:HIS:ND1	2:V:107:MET:HE2	2.32	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
2:P:221:LYS:O	2:P:222:SER:C	2.59	0.45
2:V:62:ASP:C	2:V:64:VAL:H	2.25	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:K:185:LEU:C	2:K:185:LEU:HD12	2.42	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
1:Q:4:MET:HE3	1:Q:23:CYS:SG	2.56	0.44
2:H:52:THR:HG23	2:H:53:PRO:HD2	1.99	0.44
2:B:64:VAL:HG13	2:B:68:PHE:HB2	2.00	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:G:143:GLU:CD	1:G:143:GLU:H	2.25	0.44
2:P:40:ALA:O	2:P:41:PRO:C	2.61	0.44
1:U:47:LEU:HA	1:U:58:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:108:ARG:HD3	1:U:109:THR:O	2.17	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:HH11	2:R:87:ARG:HB2	1.83	0.44
1:Q:22:THR:HG22	1:Q:72:THR:HG22	2.00	0.44
1:Q:181:LEU:HD13	1:Q:185:ASP:HB3	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:37:GLN:HB2	1:S:47:LEU:HD11	2.00	0.44
1:S:121:SER:HB2	2:T:130:PRO:HD2	1.99	0.44
1:U:198:HIS:HD2	1:U:200:GLY:H	1.65	0.44
1:G:4:MET:HE3	1:G:23:CYS:SG	2.58	0.43
1:Q:106:ILE:H	1:Q:166:GLN:HE22	1.66	0.43
2:H:185:LEU:C	2:H:185:LEU:HD12	2.42	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
1:L:163:VAL:HG22	1:L:175:LEU:HD12	2.01	0.43
2:H:28:THR:HA	2:H:77:ASN:HD21	1.84	0.43
1:S:94:THR:HG21	2:T:33:TRP:CH2	2.53	0.43
2:I:185:LEU:HD12	2:I:185:LEU:C	2.44	0.43
2:I:211:ASN:HB2	2:N:11:LEU:HD13	1.99	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
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
2:F:102:PHE:CD1	2:N:72:ALA:HB3	2.54	0.43
1:M:121:SER:O	1:M:125:LEU:HD13	2.19	0.43
1:W:4:MET:HE3	1:W:23:CYS:SG	2.59	0.43
1:G:140:TYR:CG	1:G:141:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:TYR:CZ	1:G:211:ARG:HG3	2.54	0.43
1:G:207:LYS:HD3	1:G:207:LYS:HA	1.82	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
1:J:143:GLU:CD	1:J:143:GLU:H	2.27	0.42
2:K:35:HIS:ND1	2:K:107:MET:HE2	2.34	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:HD13	1:S:106:ILE:HA	1.60	0.42
1:S:160:GLN:HE21	1:S:160:GLN:HB2	1.67	0.42
1:L:108:ARG:HD3	1:L:109:THR:O	2.19	0.42
2:F:67:ARG:C	2:F:68:PHE:HD1	2.27	0.42
2:N:89:GLU:CD	2:N:89:GLU:H	2.27	0.42
2:H:35:HIS:CD2	2:H:47:TRP:NE1	2.82	0.42
2:H:162:ASN:HA	2:H:202:ILE:HG13	2.00	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:O:159:SER:HA	1:O:178:THR:O	2.20	0.42
1:Q:165:GLU:O	1:Q:166:GLN:C	2.63	0.42
2:R:52:THR:HB	2:R:57:TYR:H	1.83	0.42
2:H:154:PRO:O	2:H:207:HIS:CE1	2.61	0.42
1:C:83:PHE:HZ	1:C:165:GLU:HG2	1.84	0.42
2:D:4:LEU:O	2:D:111:GLY:HA2	2.20	0.42
2:D:100:VAL:HG13	2:D:102:PHE:H	1.85	0.42
1:O:140:TYR:CG	1:O:141:PRO:HA	2.54	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:E:4:MET:HE3	1:E:23:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:170:ASP:C	1:J:170:ASP:OD1	2.63	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
1:Q:124:GLN:HG3	2:R:129:PHE:CE2	2.55	0.41
1:Q:187:GLU:HA	1:Q:211:ARG:NH2	2.36	0.41
2:H:83:MET:HE1	2:H:94:TYR:CZ	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
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
2:X:83:MET:HE2	2:X:86:LEU:HD21	2.01	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
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:24:ARG:HA	1:E:69:THR:O	2.21	0.41
1:E:189:HIS:O	1:E:211:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:178:GLN:C	2:I:180:SER:N	2.79	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:HD12	2:F:29:ILE:N	2.36	0.41
2:P:219:GLU:HB2	2:P:220:PRO:CD	2.51	0.41
2:T:29:ILE:H	2:T:77:ASN:HD21	1.69	0.41
2:T:154:PRO:HD2	2:T:209:PRO:CB	2.50	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
2:D:185:LEU:C	2:D:185:LEU:HD12	2.46	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:33:TRP:CD1	2:R:53:PRO:HD3	2.57	0.40
2:R:37:VAL:HG22	2:R:47:TRP:HA	2.02	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
1:Q:89:GLN:HE21	1:Q:89:GLN:HB3	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:L:7:SER:HA	1:L:8:PRO:HA	1.83	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
2:N:125:GLY:HA2	2:N:207:HIS:HD2	1.87	0.40
1:U:38:GLN:HA	3:U:224:HOH:O	2.20	0.40
1:U:142:ARG:HG2	1:U:142:ARG:HH11	1.85	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%)	12	20
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%)	24	39
1	M	209/214 (98%)	197 (94%)	9 (4%)	3 (1%)	9	14
1	O	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
1	Q	209/214 (98%)	199 (95%)	8 (4%)	2 (1%)	12	20
1	S	209/214 (98%)	201 (96%)	6 (3%)	2 (1%)	12	20
1	U	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
1	W	209/214 (98%)	197 (94%)	11 (5%)	1 (0%)	24	39
2	B	214/227 (94%)	206 (96%)	8 (4%)	0	100	100
2	D	214/227 (94%)	203 (95%)	10 (5%)	1 (0%)	24	39
2	F	214/227 (94%)	203 (95%)	9 (4%)	2 (1%)	14	24
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%)	14	24
2	R	214/227 (94%)	203 (95%)	9 (4%)	2 (1%)	14	24
2	T	214/227 (94%)	204 (95%)	8 (4%)	2 (1%)	14	24
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%)	30	45

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 ⓘ

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%)	137 (74%)	49 (26%)	0	0
1	C	186/188 (99%)	150 (81%)	36 (19%)	1	2
1	E	186/188 (99%)	157 (84%)	29 (16%)	2	3
1	G	186/188 (99%)	158 (85%)	28 (15%)	3	4
1	J	186/188 (99%)	151 (81%)	35 (19%)	1	2
1	L	186/188 (99%)	152 (82%)	34 (18%)	2	2
1	M	186/188 (99%)	141 (76%)	45 (24%)	1	0
1	O	186/188 (99%)	149 (80%)	37 (20%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	186/188 (99%)	142 (76%)	44 (24%)	1	0
1	S	186/188 (99%)	141 (76%)	45 (24%)	1	0
1	U	186/188 (99%)	141 (76%)	45 (24%)	1	0
1	W	186/188 (99%)	135 (73%)	51 (27%)	0	0
2	B	179/187 (96%)	140 (78%)	39 (22%)	1	1
2	D	179/187 (96%)	152 (85%)	27 (15%)	3	4
2	F	179/187 (96%)	144 (80%)	35 (20%)	1	2
2	H	179/187 (96%)	144 (80%)	35 (20%)	1	2
2	I	179/187 (96%)	146 (82%)	33 (18%)	1	2
2	K	179/187 (96%)	148 (83%)	31 (17%)	2	2
2	N	179/187 (96%)	143 (80%)	36 (20%)	1	1
2	P	179/187 (96%)	154 (86%)	25 (14%)	3	5
2	R	179/187 (96%)	142 (79%)	37 (21%)	1	1
2	T	179/187 (96%)	140 (78%)	39 (22%)	1	1
2	V	179/187 (96%)	147 (82%)	32 (18%)	2	2
2	X	179/187 (96%)	140 (78%)	39 (22%)	1	1
All	All	4380/4500 (97%)	3494 (80%)	886 (20%)	1	1

All (886) 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	39	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	103	LYS
1	L	105	GLU
1	L	108	ARG
1	L	114	SER

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Mol	Chain	Res	Type
1	L	117	ILE
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	187	GLU
1	L	197	THR
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	29	ILE
2	H	43	LYS
2	H	52	THR
2	H	58	THR
2	H	64	VAL
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	158	THR
2	H	176	VAL
2	H	177	LEU

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Mol	Chain	Res	Type
2	H	182	LEU
2	H	188	VAL
2	H	190	THR
2	H	194	SER
2	H	196	LEU
2	H	198	THR
2	H	199	GLN
2	H	200	THR
2	H	208	LYS
2	H	216	LYS
2	H	217	LYS
2	H	221	LYS
1	A	3	GLN
1	A	6	GLN
1	A	9	SER
1	A	10	SER
1	A	11	LEU
1	A	14	SER
1	A	18	ARG
1	A	22	THR
1	A	24	ARG
1	A	27	GLN
1	A	30	SER
1	A	42	LYS
1	A	45	LYS
1	A	48	ILE
1	A	56	SER
1	A	72	THR
1	A	73	LEU
1	A	74	THR
1	A	77	SER
1	A	83	PHE
1	A	89	GLN
1	A	93	THR
1	A	105	GLU
1	A	107	LYS
1	A	108	ARG
1	A	117	ILE
1	A	125	LEU
1	A	135	LEU
1	A	143	GLU
1	A	147	GLN

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Mol	Chain	Res	Type
1	A	151	ASP
1	A	154	LEU
1	A	164	THR
1	A	169	LYS
1	A	171	SER
1	A	177	SER
1	A	179	LEU
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
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	29	ILE
2	B	48	VAL
2	B	51	ILE
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

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Mol	Chain	Res	Type
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	188	VAL
2	B	190	THR
2	B	193	SER
2	B	194	SER
2	B	196	LEU
2	B	199	GLN
2	B	200	THR
2	B	216	LYS
2	B	221	LYS
2	B	223	CYS
1	C	3	GLN
1	C	10	SER
1	C	14	SER
1	C	24	ARG
1	C	27	GLN
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	132	VAL
1	C	135	LEU
1	C	143	GLU
1	C	147	GLN
1	C	154	LEU
1	C	164	THR

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Mol	Chain	Res	Type
1	C	169	LYS
1	C	187	GLU
1	C	188	LYS
1	C	190	LYS
1	C	195	GLU
1	C	201	LEU
1	C	206	THR
1	C	207	LYS
1	C	210	ASN
1	C	211	ARG
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	196	LEU
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	27	GLN

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Mol	Chain	Res	Type
1	E	42	LYS
1	E	48	ILE
1	E	65	SER
1	E	73	LEU
1	E	89	GLN
1	E	93	THR
1	E	94	THR
1	E	105	GLU
1	E	108	ARG
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	169	LYS
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	48	VAL
2	F	51	ILE
2	F	52	THR
2	F	58	THR
2	F	64	VAL
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

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Mol	Chain	Res	Type
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	194	SER
2	F	196	LEU
2	F	198	THR
2	F	199	GLN
2	F	208	LYS
2	F	213	LYS
2	F	216	LYS
2	F	218	VAL
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	48	ILE
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	169	LYS
1	G	181	LEU
1	G	187	GLU

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Mol	Chain	Res	Type
1	G	190	LYS
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	29	ILE
2	I	48	VAL
2	I	52	THR
2	I	58	THR
2	I	62	ASP
2	I	64	VAL
2	I	65	LYS
2	I	76	LYS
2	I	87	ARG
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	158	THR
2	I	168	SER
2	I	177	LEU
2	I	179	SER
2	I	182	LEU
2	I	186	SER
2	I	206	ASN
2	I	212	THR
2	I	217	LYS
2	I	221	LYS
2	I	222	SER
2	I	223	CYS
1	J	1	ASP
1	J	3	GLN
1	J	9	SER
1	J	18	ARG
1	J	42	LYS
1	J	45	LYS

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Mol	Chain	Res	Type
1	J	48	ILE
1	J	56	SER
1	J	73	LEU
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	163	VAL
1	J	164	THR
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
1	J	210	ASN
2	K	1	GLU
2	K	11	LEU
2	K	12	VAL
2	K	17	SER
2	K	25	SER
2	K	29	ILE
2	K	52	THR
2	K	58	THR
2	K	64	VAL
2	K	76	LYS
2	K	100	VAL
2	K	112	GLN
2	K	114	THR

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Mol	Chain	Res	Type
2	K	115	LEU
2	K	117	THR
2	K	134	SER
2	K	135	SER
2	K	142	THR
2	K	145	LEU
2	K	150	LYS
2	K	158	THR
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	212	THR
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
1	M	73	LEU
1	M	74	THR
1	M	83	PHE
1	M	89	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	125	LEU
1	M	126	LYS
1	M	131	SER
1	M	134	CYS
1	M	135	LEU
1	M	137	ASN

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Mol	Chain	Res	Type
1	M	145	LYS
1	M	147	GLN
1	M	154	LEU
1	M	155	GLN
1	M	160	GLN
1	M	161	GLU
1	M	163	VAL
1	M	164	THR
1	M	168	SER
1	M	169	LYS
1	M	172	THR
1	M	176	SER
1	M	181	LEU
1	M	183	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	4	LEU
2	N	11	LEU
2	N	12	VAL
2	N	20	LEU
2	N	25	SER
2	N	29	ILE
2	N	43	LYS
2	N	52	THR
2	N	58	THR
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

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Mol	Chain	Res	Type
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	198	THR
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	24	ARG
1	O	28	ASP
1	O	39	LYS
1	O	42	LYS
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	93	THR
1	O	94	THR
1	O	103	LYS
1	O	106	ILE
1	O	107	LYS
1	O	108	ARG
1	O	114	SER
1	O	125	LEU
1	O	129	THR
1	O	132	VAL
1	O	135	LEU
1	O	143	GLU
1	O	156	SER
1	O	161	GLU

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Mol	Chain	Res	Type
1	O	164	THR
1	O	169	LYS
1	O	171	SER
1	O	195	GLU
1	O	197	THR
1	O	201	LEU
1	O	202	SER
1	O	207	LYS
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	29	ILE
2	P	43	LYS
2	P	52	THR
2	P	58	THR
2	P	64	VAL
2	P	76	LYS
2	P	89	GLU
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
2	P	221	LYS
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	42	LYS

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Mol	Chain	Res	Type
1	Q	48	ILE
1	Q	60	SER
1	Q	72	THR
1	Q	73	LEU
1	Q	89	GLN
1	Q	93	THR
1	Q	100	GLN
1	Q	105	GLU
1	Q	106	ILE
1	Q	107	LYS
1	Q	108	ARG
1	Q	109	THR
1	Q	110	VAL
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	132	VAL
1	Q	135	LEU
1	Q	143	GLU
1	Q	145	LYS
1	Q	151	ASP
1	Q	154	LEU
1	Q	160	GLN
1	Q	161	GLU
1	Q	163	VAL
1	Q	164	THR
1	Q	169	LYS
1	Q	183	LYS
1	Q	190	LYS
1	Q	199	GLN
1	Q	201	LEU
1	Q	205	VAL
1	Q	207	LYS
1	Q	211	ARG
2	R	1	GLU
2	R	4	LEU
2	R	11	LEU
2	R	12	VAL
2	R	19	ARG

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Mol	Chain	Res	Type
2	R	20	LEU
2	R	25	SER
2	R	29	ILE
2	R	46	GLU
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	2	ILE
1	S	3	GLN
1	S	5	THR
1	S	7	SER
1	S	10	SER
1	S	11	LEU
1	S	18	ARG
1	S	19	VAL
1	S	22	THR

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Mol	Chain	Res	Type
1	S	27	GLN
1	S	42	LYS
1	S	48	ILE
1	S	56	SER
1	S	73	LEU
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	108	ARG
1	S	114	SER
1	S	121	SER
1	S	122	ASP
1	S	125	LEU
1	S	135	LEU
1	S	142	ARG
1	S	143	GLU
1	S	145	LYS
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	188	LYS
1	S	195	GLU
1	S	199	GLN
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

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Mol	Chain	Res	Type
2	T	43	LYS
2	T	51	ILE
2	T	52	THR
2	T	58	THR
2	T	62	ASP
2	T	64	VAL
2	T	76	LYS
2	T	87	ARG
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	145	LEU
2	T	157	VAL
2	T	158	THR
2	T	167	THR
2	T	168	SER
2	T	177	LEU
2	T	179	SER
2	T	182	LEU
2	T	188	VAL
2	T	194	SER
2	T	199	GLN
2	T	208	LYS
2	T	213	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	48	ILE
1	U	52	SER
1	U	56	SER

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Mol	Chain	Res	Type
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	109	THR
1	U	114	SER
1	U	117	ILE
1	U	123	GLU
1	U	125	LEU
1	U	131	SER
1	U	135	LEU
1	U	142	ARG
1	U	143	GLU
1	U	145	LYS
1	U	147	GLN
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	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	205	VAL
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	29	ILE
2	V	51	ILE

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Mol	Chain	Res	Type
2	V	52	THR
2	V	57	TYR
2	V	58	THR
2	V	64	VAL
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	155	GLU
2	V	157	VAL
2	V	158	THR
2	V	176	VAL
2	V	177	LEU
2	V	188	VAL
2	V	193	SER
2	V	198	THR
2	V	199	GLN
2	V	213	LYS
2	V	216	LYS
2	V	221	LYS
1	W	1	ASP
1	W	3	GLN
1	W	5	THR
1	W	6	GLN
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	81	GLU
1	W	83	PHE
1	W	91	SER
1	W	93	THR
1	W	94	THR

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Mol	Chain	Res	Type
1	W	105	GLU
1	W	106	ILE
1	W	107	LYS
1	W	108	ARG
1	W	110	VAL
1	W	117	ILE
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	154	LEU
1	W	161	GLU
1	W	164	THR
1	W	165	GLU
1	W	168	SER
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	199	GLN
1	W	201	LEU
1	W	205	VAL
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	25	SER
2	X	29	ILE
2	X	52	THR
2	X	58	THR

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Mol	Chain	Res	Type
2	X	64	VAL
2	X	65	LYS
2	X	77	ASN
2	X	87	ARG
2	X	91	THR
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	145	LEU
2	X	150	LYS
2	X	168	SER
2	X	177	LEU
2	X	179	SER
2	X	182	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	202	ILE
2	X	208	LYS
2	X	216	LYS
2	X	221	LYS
2	X	222	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	79	GLN
1	L	138	ASN
1	L	152	ASN
1	L	158	ASN
1	L	160	GLN
1	L	198	HIS
1	L	199	GLN

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Mol	Chain	Res	Type
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	160	GLN
1	A	198	HIS
2	B	162	ASN
2	B	207	HIS
1	C	27	GLN
1	C	160	GLN
1	C	189	HIS
1	C	198	HIS
1	C	199	GLN
2	D	171	HIS
2	D	207	HIS
1	E	37	GLN
1	E	79	GLN
1	E	89	GLN
1	E	160	GLN
1	E	198	HIS
1	E	210	ASN
2	F	3	GLN
2	F	82	GLN
2	F	206	ASN
2	F	207	HIS
1	G	3	GLN
1	G	79	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	82	GLN
2	I	162	ASN
2	I	199	GLN
2	I	207	HIS
1	J	3	GLN
1	J	37	GLN
1	J	89	GLN

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Mol	Chain	Res	Type
1	J	160	GLN
1	J	198	HIS
2	K	77	ASN
2	K	82	GLN
2	K	84	ASN
2	K	206	ASN
2	K	207	HIS
1	M	89	GLN
1	M	124	GLN
1	M	160	GLN
1	M	198	HIS
1	M	199	GLN
2	N	13	GLN
2	N	82	GLN
2	N	84	ASN
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	189	HIS
1	O	198	HIS
1	O	199	GLN
1	O	210	ASN
2	P	35	HIS
2	P	77	ASN
2	P	162	ASN
2	P	178	GLN
1	Q	79	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

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Mol	Chain	Res	Type
1	S	79	GLN
1	S	89	GLN
1	S	90	GLN
1	S	124	GLN
1	S	137	ASN
1	S	160	GLN
1	S	198	HIS
1	S	210	ASN
2	T	77	ASN
2	T	82	GLN
2	T	84	ASN
2	T	162	ASN
2	T	207	HIS
1	U	38	GLN
1	U	79	GLN
1	U	89	GLN
1	U	124	GLN
1	U	137	ASN
1	U	152	ASN
1	U	160	GLN
1	U	189	HIS
1	U	198	HIS
1	U	210	ASN
2	V	3	GLN
2	V	39	GLN
2	V	77	ASN
2	V	82	GLN
2	V	84	ASN
2	V	162	ASN
2	V	206	ASN
2	V	207	HIS
1	W	137	ASN
1	W	138	ASN
1	W	198	HIS
2	X	3	GLN
2	X	35	HIS
2	X	77	ASN
2	X	162	ASN
2	X	206	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	211/214 (98%)	0.13	2 (0%) 81 78	5, 11, 14, 17	0
1	C	211/214 (98%)	-0.06	4 (1%) 66 61	5, 11, 14, 16	0
1	E	211/214 (98%)	-0.08	1 (0%) 87 85	7, 11, 13, 15	0
1	G	211/214 (98%)	-0.45	1 (0%) 87 85	4, 10, 14, 17	0
1	J	211/214 (98%)	0.03	12 (5%) 29 23	6, 10, 13, 18	0
1	L	211/214 (98%)	0.86	34 (16%) 4 3	5, 11, 14, 16	0
1	M	211/214 (98%)	1.19	63 (29%) 1 0	7, 10, 13, 16	0
1	O	211/214 (98%)	0.02	16 (7%) 20 15	6, 11, 14, 17	0
1	Q	211/214 (98%)	0.31	6 (2%) 55 48	6, 11, 13, 15	0
1	S	211/214 (98%)	0.09	5 (2%) 59 53	7, 11, 13, 15	0
1	U	211/214 (98%)	0.21	13 (6%) 26 20	7, 11, 14, 15	0
1	W	211/214 (98%)	0.53	13 (6%) 26 20	7, 10, 13, 14	0
2	B	218/227 (96%)	-0.39	2 (0%) 81 78	6, 10, 14, 20	0
2	D	218/227 (96%)	-0.23	6 (2%) 55 48	5, 10, 14, 19	0
2	F	218/227 (96%)	-0.09	5 (2%) 61 54	6, 10, 14, 19	0
2	H	218/227 (96%)	0.23	26 (11%) 9 7	5, 10, 14, 20	0
2	I	218/227 (96%)	-0.54	3 (1%) 73 69	6, 10, 14, 22	0
2	K	218/227 (96%)	-0.43	3 (1%) 73 69	5, 10, 15, 22	0
2	N	218/227 (96%)	1.05	70 (32%) 1 0	4, 11, 13, 22	0
2	P	218/227 (96%)	-0.64	1 (0%) 87 85	5, 10, 14, 22	0
2	R	218/227 (96%)	-0.27	2 (0%) 81 78	6, 10, 13, 23	0
2	T	218/227 (96%)	-0.35	1 (0%) 87 85	6, 10, 14, 21	0
2	V	218/227 (96%)	-0.41	1 (0%) 87 85	3, 10, 14, 22	0
2	X	218/227 (96%)	0.12	3 (1%) 73 69	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%)	0.03	293 (5%)	29	23	3, 10, 14, 23	0

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	122	SER	14.3
2	N	179	SER	7.1
2	N	123	THR	6.9
1	M	157	GLY	6.9
1	J	168	SER	6.5
2	N	153	PHE	6.4
2	N	209	PRO	6.3
2	N	141	GLY	6.1
2	H	223	CYS	6.1
1	M	156	SER	6.0
2	N	201	TYR	5.8
2	N	175	ALA	5.8
2	N	211	ASN	5.8
2	F	222	SER	5.7
2	N	155	GLU	5.7
2	N	132	ALA	5.5
1	U	168	SER	5.5
2	N	156	PRO	5.3
2	V	223	CYS	5.3
1	M	181	LEU	5.2
2	N	125	GLY	5.1
1	M	165	GLU	5.1
2	N	180	SER	5.1
2	N	218	VAL	4.9
2	I	223	CYS	4.9
2	N	154	PRO	4.8
2	N	130	PRO	4.8
2	N	207	HIS	4.7
1	M	143	GLU	4.6
1	O	168	SER	4.6
2	N	152	TYR	4.6
1	U	171	SER	4.6
2	H	195	SER	4.6
1	M	140	TYR	4.4
1	M	83	PHE	4.4
2	H	154	PRO	4.3
2	N	210	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	M	194	CYS	4.2
2	N	183	TYR	4.2
2	N	184	SER	4.2
1	M	209	PHE	4.2
2	N	198	THR	4.2
1	M	122	ASP	4.1
2	N	150	LYS	4.1
1	O	184	ALA	4.0
1	M	158	ASN	4.0
1	M	163	VAL	4.0
2	N	157	VAL	4.0
2	N	182	LEU	4.0
1	M	155	GLN	3.9
2	F	223	CYS	3.9
2	N	145	LEU	3.9
2	N	223	CYS	3.9
2	N	144	ALA	3.9
2	N	212	THR	3.8
1	L	209	PHE	3.8
1	L	165	GLU	3.8
2	N	148	LEU	3.8
2	N	185	LEU	3.7
2	B	222	SER	3.7
2	N	174	PRO	3.7
2	N	149	VAL	3.6
2	N	192	PRO	3.6
2	H	153	PHE	3.6
1	J	169	LYS	3.6
2	H	132	ALA	3.6
2	N	124	LYS	3.6
1	W	105	GLU	3.5
2	N	181	GLY	3.5
2	H	122	SER	3.5
1	M	160	GLN	3.5
1	M	159	SER	3.5
1	M	147	GLN	3.5
1	W	106	ILE	3.4
1	L	166	GLN	3.4
2	K	223	CYS	3.4
2	H	156	PRO	3.4
1	L	157	GLY	3.4
1	M	148	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	168	SER	3.4
1	M	173	TYR	3.4
1	J	172	THR	3.4
1	L	32	ALA	3.4
2	D	223	CYS	3.4
2	H	221	LYS	3.3
2	N	208	LYS	3.3
2	N	177	LEU	3.3
2	N	191	VAL	3.3
2	N	190	THR	3.3
1	M	119	PRO	3.3
1	M	154	LEU	3.3
1	J	171	SER	3.3
1	M	153	ALA	3.3
2	H	191	VAL	3.3
1	L	105	GLU	3.2
1	M	204	PRO	3.2
1	M	145	LYS	3.2
2	F	168	SER	3.2
2	N	127	SER	3.2
1	M	180	THR	3.2
1	M	116	PHE	3.2
2	N	151	ASP	3.2
2	N	213	LYS	3.2
2	N	178	GLN	3.2
2	B	223	CYS	3.2
1	M	115	VAL	3.2
1	U	110	VAL	3.2
1	L	171	SER	3.1
1	O	170	ASP	3.1
2	N	196	LEU	3.1
2	H	144	ALA	3.1
2	N	131	LEU	3.1
1	M	166	GLN	3.1
1	M	144	ALA	3.1
1	M	110	VAL	3.1
2	N	135	SER	3.1
2	H	123	THR	3.0
1	U	210	ASN	3.0
1	W	12	SER	3.0
1	W	1	ASP	3.0
2	H	158	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	121	SER	2.9
1	M	161	GLU	2.9
1	U	138	ASN	2.9
1	L	192	TYR	2.9
1	M	192	TYR	2.9
2	R	141	GLY	2.9
1	M	120	PRO	2.9
2	N	199	GLN	2.9
1	M	179	LEU	2.9
1	U	165	GLU	2.9
1	M	105	GLU	2.8
1	M	168	SER	2.8
2	X	223	CYS	2.8
1	L	93	THR	2.8
1	M	129	THR	2.8
2	N	142	THR	2.8
2	N	126	PRO	2.8
2	D	122	SER	2.8
1	O	171	SER	2.8
2	X	134	SER	2.8
2	N	146	GLY	2.8
1	L	106	ILE	2.8
2	N	195	SER	2.8
1	M	191	VAL	2.8
1	A	80	PRO	2.7
2	T	179	SER	2.7
1	M	1	ASP	2.7
1	U	111	ALA	2.7
2	N	129	PHE	2.7
1	L	50	SER	2.7
1	M	171	SER	2.7
2	H	222	SER	2.7
1	W	169	LYS	2.7
2	H	152	TYR	2.7
2	K	222	SER	2.7
1	O	165	GLU	2.7
2	N	206	ASN	2.7
2	H	135	SER	2.7
1	J	154	LEU	2.6
1	J	138	ASN	2.6
2	H	134	SER	2.6
1	M	93	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	183	LYS	2.6
2	N	221	LYS	2.6
1	L	163	VAL	2.6
1	L	92	TYR	2.6
1	L	153	ALA	2.6
1	W	91	SER	2.6
2	N	216	LYS	2.6
1	L	184	ALA	2.6
1	J	163	VAL	2.6
2	N	176	VAL	2.6
1	L	167	ASP	2.5
1	U	167	ASP	2.5
1	Q	110	VAL	2.5
1	M	199	GLN	2.5
1	U	166	GLN	2.5
1	O	172	THR	2.5
1	L	140	TYR	2.5
2	N	189	VAL	2.5
1	L	130	ALA	2.5
2	X	211	ASN	2.5
1	S	168	SER	2.5
1	O	169	LYS	2.5
1	Q	148	TRP	2.5
1	S	184	ALA	2.5
1	O	137	ASN	2.5
1	E	171	SER	2.5
1	Q	171	SER	2.5
1	W	77	SER	2.5
2	H	210	SER	2.5
1	L	1	ASP	2.5
1	L	55	TYR	2.5
2	H	183	TYR	2.5
1	O	166	GLN	2.5
2	N	200	THR	2.4
1	L	162	SER	2.4
2	F	156	PRO	2.4
1	O	110	VAL	2.4
1	U	190	LYS	2.4
2	D	123	THR	2.4
1	M	152	ASN	2.4
1	M	131	SER	2.4
1	L	151	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	N	217	LYS	2.4
1	O	192	TYR	2.4
1	M	189	HIS	2.4
2	N	169	GLY	2.4
2	D	177	LEU	2.4
1	O	150	VAL	2.4
1	M	184	ALA	2.4
1	M	164	THR	2.3
1	M	80	PRO	2.3
1	W	93	THR	2.3
1	C	168	SER	2.3
1	J	167	ASP	2.3
1	J	170	ASP	2.3
1	M	185	ASP	2.3
1	Q	153	ALA	2.3
2	H	207	HIS	2.3
1	W	94	THR	2.3
1	L	195	GLU	2.3
2	H	124	LYS	2.3
1	S	171	SER	2.3
2	N	194	SER	2.3
1	J	184	ALA	2.3
1	M	193	ALA	2.3
2	N	165	ALA	2.3
1	L	169	LYS	2.3
1	S	170	ASP	2.3
1	U	170	ASP	2.3
2	D	179	SER	2.3
1	M	79	GLN	2.3
1	L	150	VAL	2.3
1	L	83	PHE	2.3
2	P	223	CYS	2.2
1	U	169	LYS	2.2
1	C	93	THR	2.2
1	M	176	SER	2.2
2	N	214	VAL	2.2
1	W	109	THR	2.2
2	F	169	GLY	2.2
1	O	181	LEU	2.2
1	L	111	ALA	2.2
1	L	164	THR	2.2
1	M	175	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	83	PHE	2.2
1	Q	165	GLU	2.2
1	Q	113	PRO	2.2
1	U	140	TYR	2.2
2	H	192	PRO	2.2
2	I	221	LYS	2.2
1	M	132	VAL	2.2
2	K	135	SER	2.2
2	N	168	SER	2.2
2	N	186	SER	2.2
2	N	222	SER	2.2
1	M	142	ARG	2.1
1	O	142	ARG	2.1
2	H	196	LEU	2.1
2	H	163	SER	2.1
1	J	164	THR	2.1
1	M	178	THR	2.1
1	M	141	PRO	2.1
1	O	138	ASN	2.1
1	L	94	THR	2.1
1	M	206	THR	2.1
2	I	197	GLY	2.1
1	L	174	SER	2.1
1	C	153	ALA	2.1
2	H	142	THR	2.1
1	M	135	LEU	2.1
1	S	181	LEU	2.1
2	R	197	GLY	2.1
1	L	173	TYR	2.1
1	M	196	VAL	2.1
1	C	1	ASP	2.0
2	N	1	GLU	2.0
1	M	208	SER	2.0
1	W	168	SER	2.0
2	H	133	PRO	2.0
2	D	197	GLY	2.0
1	O	167	ASP	2.0
1	J	162	SER	2.0
2	N	193	SER	2.0
1	L	3	GLN	2.0
1	G	2	ILE	2.0
1	W	57	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	141	GLY	2.0
1	L	110	VAL	2.0
1	W	104	VAL	2.0
1	M	92	TYR	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.