



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:58 PM UTC

PDB ID : 6N16 / pdb_00006n16
Title : Vaccine-elicited NHP FP-targeting neutralizing antibody 0PV-b.01 in complex with HIV fusion peptide (residue 512-519)
Authors : Xu, K.; Wang, Y.; Kwong, P.D.
Deposited on : 2018-11-08
Resolution : 2.30 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

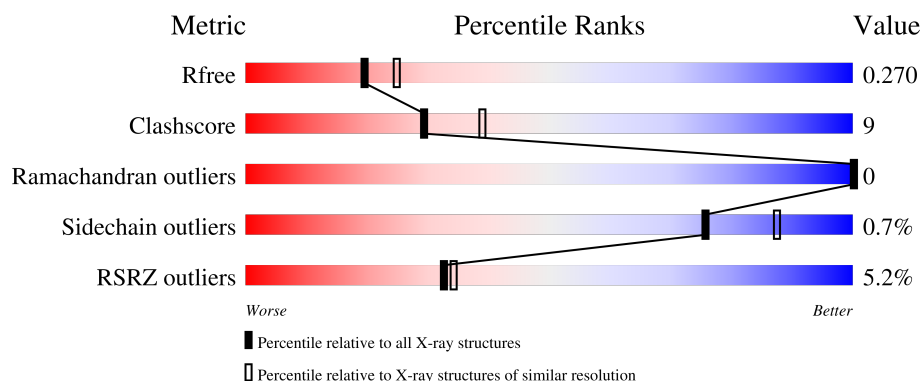
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



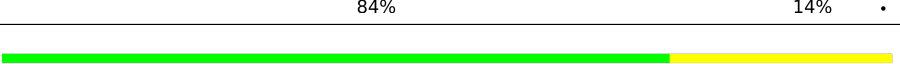
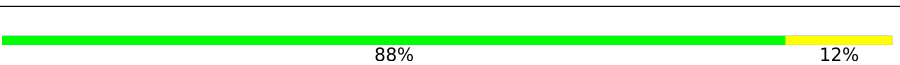
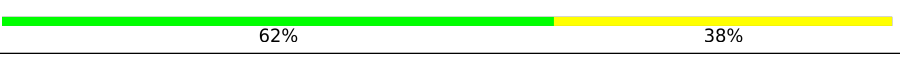
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	223	3% 87% 9% ..
1	C	223	4% 72% 25% ..
1	H	223	4% 81% 17% ..
1	K	223	4% 78% 19% .
2	B	217	3% 81% 18% .

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Mol	Chain	Length	Quality of chain
2	D	217	
2	J	217	
2	L	217	
3	E	8	
3	F	8	
3	G	8	
3	I	8	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13377 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 antibody 0PV-b.01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1622	1027	271	320	4			
1	H	219	Total	C	N	O	S	0	0	0
			1637	1035	273	325	4			
1	K	219	Total	C	N	O	S	0	0	0
			1637	1035	273	325	4			
1	C	219	Total	C	N	O	S	0	0	0
			1637	1035	273	325	4			

- Molecule 2 is a protein called antibody 0PV-b.01 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1660	1039	280	336	5			
2	J	217	Total	C	N	O	S	0	0	0
			1660	1039	280	336	5			
2	L	217	Total	C	N	O	S	0	0	0
			1660	1039	280	336	5			
2	D	217	Total	C	N	O	S	0	0	0
			1660	1039	280	336	5			

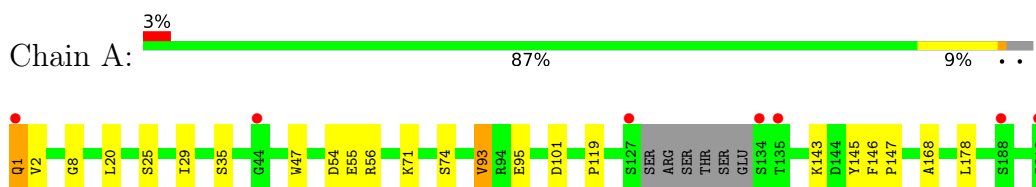
- Molecule 3 is a protein called HIV fusion peptide (512-519).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	0	0	0
			51	35	8	8			
3	F	8	Total	C	N	O	0	0	0
			51	35	8	8			
3	G	8	Total	C	N	O	0	0	0
			51	35	8	8			
3	I	8	Total	C	N	O	0	0	0
			51	35	8	8			

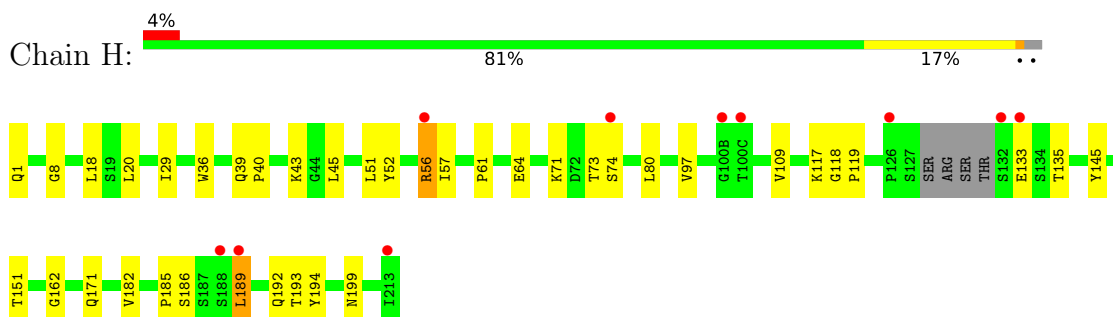
3 Residue-property plots [i](#)

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.

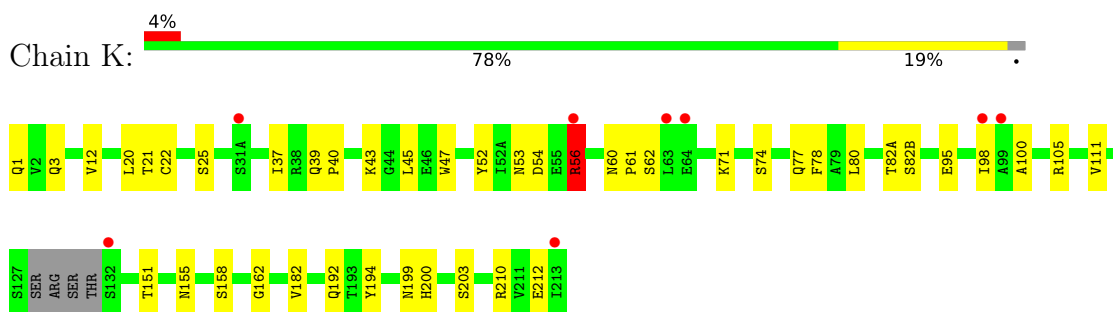
- Molecule 1: antibody 0PV-b.01 Fab heavy chain



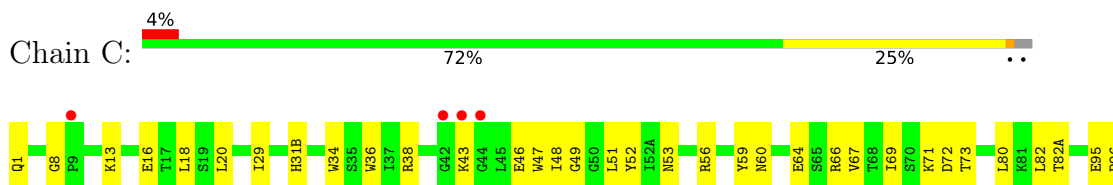
- Molecule 1: antibody 0PV-b.01 Fab heavy chain



- Molecule 1: antibody 0PV-b.01 Fab heavy chain

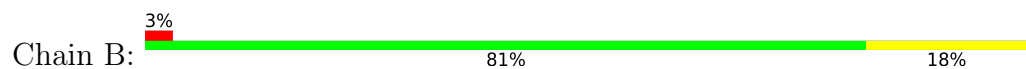


- Molecule 1: antibody 0PV-b.01 Fab heavy chain

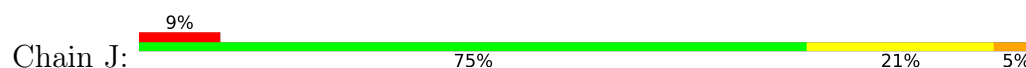




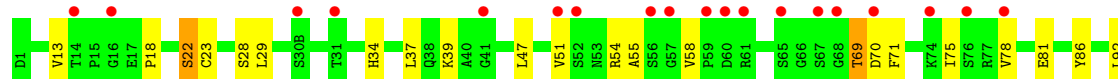
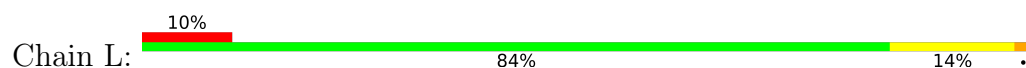
- Molecule 2: antibody 0PV-b.01 Fab light chain



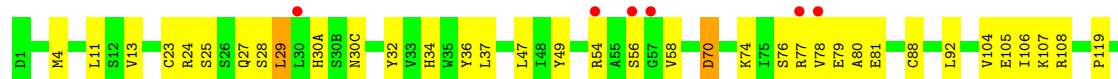
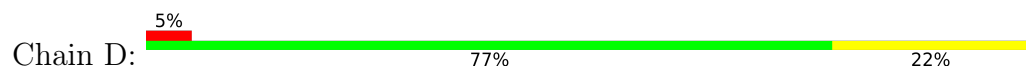
- Molecule 2: antibody 0PV-b.01 Fab light chain



- Molecule 2: antibody 0PV-b.01 Fab light chain



- Molecule 2: antibody 0PV-b.01 Fab light chain



- Molecule 3: HIV fusion peptide (512-519)

Chain E:  75% 25%



- Molecule 3: HIV fusion peptide (512-519)

Chain F:  88% 12%



- Molecule 3: HIV fusion peptide (512-519)

Chain G:  62% 38%



- Molecule 3: HIV fusion peptide (512-519)

Chain I:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.50Å 84.20Å 84.57Å 89.88° 111.43° 104.48°	Depositor
Resolution (Å)	43.07 – 2.30 43.07 – 2.30	Depositor EDS
% Data completeness (in resolution range)	85.0 (43.07-2.30) 84.9 (43.07-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.222 , 0.274 (Not available) , 0.270	Depositor DCC
R_{free} test set	3358 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13377	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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	0.35	0/1660	0.64	2/2272 (0.1%)
1	C	0.54	3/1675 (0.2%)	0.67	3/2292 (0.1%)
1	H	0.35	0/1675	0.72	4/2292 (0.2%)
1	K	0.31	0/1675	0.70	4/2292 (0.2%)
2	B	0.65	6/1696 (0.4%)	0.68	2/2306 (0.1%)
2	D	0.69	6/1696 (0.4%)	0.76	3/2306 (0.1%)
2	J	0.88	11/1696 (0.6%)	0.88	12/2306 (0.5%)
2	L	0.70	4/1696 (0.2%)	0.77	4/2306 (0.2%)
3	E	0.28	0/51	0.62	0/68
3	F	0.20	0/51	0.42	0/68
3	G	0.20	0/51	0.40	0/68
3	I	1.89	2/51 (3.9%)	1.03	0/68
All	All	0.60	32/13673 (0.2%)	0.73	34/18644 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1
2	D	0	1
All	All	0	2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	33	VAL	C-O	-9.04	1.15	1.24
2	B	28	SER	C-O	-8.30	1.14	1.23
2	J	66	GLY	C-O	-7.52	1.17	1.23
2	J	67	SER	C-O	-7.07	1.15	1.24
2	D	25	SER	C-O	-6.89	1.15	1.23
2	J	67	SER	CA-C	-6.84	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	96	PRO	C-O	-6.72	1.16	1.23
2	D	28	SER	C-O	-6.57	1.15	1.23
2	B	27	GLN	C-O	-6.29	1.16	1.23
2	B	70	ASP	C-O	-6.29	1.16	1.24
2	D	70	ASP	C-O	-6.15	1.17	1.24
2	J	66	GLY	CA-C	-6.11	1.45	1.52
2	L	23	CYS	C-O	-6.05	1.17	1.24
2	B	67	SER	C-O	-5.98	1.16	1.23
2	D	29	LEU	C-O	-5.96	1.15	1.24
2	J	25	SER	CA-C	-5.90	1.45	1.52
3	I	516	GLY	C-O	-5.90	1.16	1.23
1	C	97	VAL	C-O	-5.75	1.16	1.24
2	D	27	GLN	C-O	-5.75	1.16	1.23
2	L	119	PRO	CA-C	-5.72	1.48	1.52
2	B	69	THR	C-O	-5.71	1.16	1.24
2	J	48	ILE	C-O	-5.64	1.18	1.24
2	D	27	GLN	CA-C	-5.53	1.45	1.52
2	L	70	ASP	CA-C	-5.46	1.46	1.52
3	I	515	ILE	C-O	-5.46	1.18	1.24
2	J	29	LEU	CA-C	-5.38	1.45	1.52
2	B	30	LEU	C-O	-5.37	1.17	1.24
2	J	154	LEU	CG-CD2	5.37	1.70	1.52
2	J	25	SER	C-O	-5.22	1.17	1.23
1	C	135	THR	C-O	-5.14	1.18	1.23
2	J	53	ASN	C-O	-5.13	1.17	1.23
2	L	22	SER	C-O	-5.12	1.17	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	56	ARG	CG-CD-NE	11.15	136.54	112.00
1	K	56	ARG	NE-CZ-NH1	-10.45	111.05	121.50
2	J	185	GLU	CA-CB-CG	-10.42	93.25	114.10
1	K	56	ARG	CD-NE-CZ	9.95	138.33	124.40
2	J	68	GLY	N-CA-C	7.74	122.27	112.83
1	H	56	ARG	CA-CB-CG	-7.72	98.65	114.10
1	H	133	GLU	CA-CB-CG	7.17	128.43	114.10
1	H	56	ARG	CB-CG-CD	6.95	127.29	111.30
2	D	32	TYR	N-CA-C	6.70	119.99	110.68
2	B	24	ARG	CA-CB-CG	-6.67	100.77	114.10
2	L	190	LYS	CD-CE-NZ	-6.55	90.94	111.90
2	L	119	PRO	O-C-N	-6.47	118.11	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	126	LYS	CB-CG-CD	-6.22	96.99	111.30
1	K	56	ARG	CB-CG-CD	6.13	125.39	111.30
2	L	69	THR	N-CA-C	5.83	119.71	112.59
1	A	1	GLN	CA-CB-CG	5.68	125.47	114.10
2	D	54	ARG	NE-CZ-NH1	-5.43	116.07	121.50
2	J	52	SER	N-CA-C	5.43	121.75	113.61
1	C	212	GLU	CG-CD-OE1	-5.40	105.98	118.40
1	A	93	VAL	CG1-CB-CG2	5.38	122.62	110.80
2	B	24	ARG	CB-CA-C	5.34	119.93	109.35
2	J	54	ARG	N-CA-CB	5.30	119.27	110.52
2	J	51	VAL	N-CA-C	5.29	120.33	109.34
2	J	68	GLY	CA-C-O	-5.24	115.67	120.80
2	J	67	SER	CA-C-N	5.19	125.85	120.03
2	J	67	SER	C-N-CA	5.19	125.85	120.03
2	D	126	LYS	CA-CB-CG	5.19	124.47	114.10
2	J	125	VAL	CA-C-N	-5.17	112.08	120.72
2	J	125	VAL	C-N-CA	-5.17	112.08	120.72
1	H	189	LEU	N-CA-CB	-5.16	102.27	110.22
1	C	95	GLU	CA-C-N	-5.10	114.66	119.76
1	C	95	GLU	C-N-CA	-5.10	114.66	119.76
2	J	169	LYS	CG-CD-CE	-5.06	99.66	111.30
2	L	147	LYS	CG-CD-CE	5.06	122.93	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	185	GLU	Sidechain
1	K	56	ARG	Sidechain

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	1622	0	1607	15	1
1	C	1637	0	1618	39	1
1	H	1637	0	1618	33	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1637	0	1618	28	1
2	B	1660	0	1616	33	1
2	D	1660	0	1616	29	1
2	J	1660	0	1616	45	0
2	L	1660	0	1616	23	0
3	E	51	0	53	3	0
3	F	51	0	53	1	0
3	G	51	0	53	3	0
3	I	51	0	53	2	0
All	All	13377	0	13137	228	3

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 9.

All (228) 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:J:11:LEU:HD21	2:J:13:VAL:HG23	1.17	1.14
1:H:56:ARG:HH22	1:K:3:GLN:HB3	1.33	0.93
2:B:24:ARG:NH2	2:B:70:ASP:OD1	2.02	0.93
1:H:71:LYS:HE2	1:H:73:THR:HG22	1.50	0.93
1:C:126:PRO:HD3	1:C:138:LEU:HD23	1.51	0.90
2:B:24:ARG:NH1	2:B:70:ASP:HB2	1.87	0.90
1:H:56:ARG:NH1	1:K:1:GLN:O	2.04	0.90
2:B:155:LYS:NZ	2:B:156:THR:O	2.09	0.86
2:J:24:ARG:NH1	2:J:70:ASP:OD1	2.08	0.85
2:B:155:LYS:HE3	2:B:157:GLY:O	1.79	0.83
1:C:31(B):HIS:H	1:C:53:ASN:HD21	1.29	0.81
2:D:24:ARG:HH22	2:D:70:ASP:HB2	1.45	0.81
2:D:36:TYR:HH	3:I:512:ALA:N	1.77	0.81
1:C:59:TYR:HB2	1:C:64:GLU:HB2	1.62	0.81
2:J:136:LEU:HD11	2:J:196:VAL:HG21	1.63	0.80
1:C:59:TYR:CB	1:C:64:GLU:HB2	2.13	0.79
1:C:126:PRO:HD3	1:C:138:LEU:CD2	2.13	0.78
2:L:105:GLU:OE1	2:L:173:TYR:OH	2.02	0.77
1:H:171:GLN:OE1	2:L:160:GLN:NE2	2.19	0.76
2:B:11:LEU:HD21	2:B:13:VAL:HG23	1.68	0.75
1:C:71:LYS:HD3	1:C:73:THR:HG23	1.70	0.74
2:B:54:ARG:NH2	2:B:62:PHE:O	2.21	0.73
1:C:126:PRO:HD2	1:C:213:ILE:HD13	1.69	0.73
2:B:11:LEU:CD2	2:B:13:VAL:HG23	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:54:ARG:NH2	2:J:60:ASP:HA	2.05	0.71
2:D:24:ARG:NH2	2:D:70:ASP:HB2	2.05	0.71
2:B:36:TYR:HH	3:E:512:ALA:N	1.91	0.69
1:H:29:ILE:HG12	1:H:71:LYS:HG3	1.74	0.69
2:J:95:PRO:HG3	1:K:61:PRO:HD2	1.74	0.68
2:J:103:LYS:NZ	2:J:104:VAL:O	2.24	0.68
2:B:59:PRO:HG3	2:B:61:ARG:HH11	1.57	0.68
2:D:105:GLU:OE1	2:D:173:TYR:OH	2.05	0.68
2:J:13:VAL:HG11	2:J:78:VAL:HB	1.75	0.68
2:L:105:GLU:OE2	2:L:140:TYR:CE1	2.47	0.67
2:L:181:LEU:HD22	2:L:185:GLU:OE2	1.93	0.67
2:B:13:VAL:HG11	2:B:78:VAL:HB	1.77	0.67
1:K:95:GLU:HG3	3:G:515:ILE:HD11	1.79	0.64
1:H:71:LYS:CE	1:H:73:THR:HG22	2.27	0.64
1:A:55:GLU:HG3	1:A:55:GLU:O	1.97	0.64
2:L:37:LEU:HB2	2:L:47:LEU:HD11	1.78	0.64
2:D:190:LYS:NZ	2:D:211:ARG:O	2.31	0.64
1:K:54:ASP:CG	1:K:56:ARG:HG3	2.21	0.64
2:B:24:ARG:HG2	2:B:69:THR:O	1.99	0.63
2:J:61:ARG:HD2	2:J:77:ARG:O	1.99	0.63
2:D:80:ALA:HA	2:D:106:ILE:HD11	1.80	0.63
2:J:11:LEU:HD23	2:J:11:LEU:C	2.23	0.63
2:L:105:GLU:OE2	2:L:140:TYR:HE1	1.82	0.62
2:D:77:ARG:NH2	2:D:79:GLU:OE1	2.31	0.62
2:J:29:LEU:CD1	2:J:33:VAL:CG1	2.78	0.62
2:J:36:TYR:HH	3:G:512:ALA:N	1.98	0.62
1:C:13:LYS:HB2	1:C:16:GLU:OE2	2.01	0.61
2:L:190:LYS:HZ1	2:L:210:ASN:HB3	1.65	0.61
2:B:181:LEU:HB3	2:B:185:GLU:HG3	1.82	0.61
2:J:11:LEU:CD2	2:J:13:VAL:HG23	2.12	0.61
2:L:190:LYS:NZ	2:L:210:ASN:HB3	2.16	0.61
1:H:192:GLN:HG2	1:H:194:TYR:CZ	2.35	0.61
2:D:183:SER:O	2:D:187:GLN:HG3	2.00	0.61
2:J:29:LEU:HD12	2:J:33:VAL:CG1	2.32	0.60
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.83	0.60
1:H:51:LEU:HD12	1:H:57:ILE:HD11	1.84	0.59
1:C:38:ARG:HD2	1:C:46:GLU:OE2	2.02	0.59
1:A:35:SER:OG	1:A:47:TRP:NE1	2.35	0.58
1:K:39:GLN:HB2	1:K:45:LEU:HD23	1.86	0.58
2:J:13:VAL:HG21	2:J:19:ALA:HB2	1.85	0.58
1:H:56:ARG:HG3	1:H:57:ILE:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31(B):HIS:H	1:C:53:ASN:ND2	1.99	0.57
1:C:43:LYS:O	1:C:43:LYS:HD3	2.03	0.57
2:J:77:ARG:HH11	2:J:79:GLU:CD	2.12	0.57
1:C:52:TYR:CE2	1:C:53:ASN:HB2	2.40	0.57
2:B:155:LYS:HE3	2:B:158:ASN:HB2	1.86	0.57
1:H:8:GLY:HA3	1:H:20:LEU:HD23	1.86	0.56
1:C:210:ARG:CZ	1:C:212:GLU:OE1	2.53	0.56
2:J:29:LEU:HD13	2:J:33:VAL:HG12	1.87	0.56
1:K:200:HIS:ND1	1:K:203:SER:HB3	2.21	0.56
2:D:105:GLU:HG2	2:D:106:ILE:N	2.20	0.56
1:H:52:TYR:CE2	1:H:97:VAL:HG11	2.41	0.56
1:C:59:TYR:HB3	1:C:64:GLU:HB2	1.86	0.55
1:C:8:GLY:HA3	1:C:20:LEU:HD23	1.88	0.55
1:A:8:GLY:HA3	1:A:20:LEU:HD23	1.89	0.55
1:A:29:ILE:HG12	1:A:71:LYS:HG3	1.88	0.55
1:H:56:ARG:NH2	1:K:3:GLN:HB3	2.14	0.55
1:H:61:PRO:HD2	2:L:95:PRO:HG3	1.87	0.55
2:D:29:LEU:HA	2:D:92:LEU:HD22	1.88	0.55
2:J:29:LEU:CD1	2:J:33:VAL:HG12	2.37	0.55
2:L:54:ARG:HB3	2:L:58:VAL:HG13	1.89	0.54
1:H:51:LEU:HB2	1:H:57:ILE:HD13	1.89	0.54
1:K:37:ILE:HD13	1:K:47:TRP:HA	1.90	0.54
1:K:98:ILE:HD12	1:K:100:ALA:HB3	1.88	0.54
2:J:67:SER:OG	2:J:68:GLY:N	2.38	0.54
1:C:188:SER:HB3	1:C:192:GLN:HG3	1.90	0.54
2:B:24:ARG:HG3	2:B:70:ASP:HA	1.89	0.54
1:C:100(C):THR:HB	2:D:56:SER:OG	2.08	0.54
2:D:154:LEU:HD21	2:D:156:THR:HG23	1.91	0.53
2:L:51:VAL:HG22	2:L:71:PHE:CE2	2.44	0.53
2:D:11:LEU:HD12	2:D:104:VAL:HG22	1.90	0.53
2:J:151:ASP:OD1	2:J:189:HIS:ND1	2.41	0.52
2:L:55:ALA:O	2:L:58:VAL:HG12	2.10	0.52
2:B:155:LYS:HD2	2:B:179:LEU:HD11	1.91	0.52
1:C:52:TYR:CE1	1:C:97:VAL:HG21	2.45	0.52
2:D:13:VAL:HG11	2:D:78:VAL:HG21	1.91	0.52
1:A:101:ASP:OD2	3:E:512:ALA:N	2.43	0.51
2:J:54:ARG:NH1	2:J:60:ASP:OD1	2.43	0.51
1:A:54:ASP:CG	1:A:56:ARG:HG3	2.35	0.51
1:H:71:LYS:NZ	1:H:73:THR:CG2	2.74	0.51
1:H:18:LEU:HD12	1:H:109:VAL:HG11	1.93	0.50
2:J:105:GLU:HG2	2:J:106:ILE:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:52:TYR:CZ	1:K:53:ASN:HB2	2.46	0.50
2:J:21:ILE:HD12	2:J:73:LEU:HD23	1.93	0.50
2:J:145:SER:HB2	2:J:197:THR:OG1	2.12	0.50
2:D:107:LYS:HE2	2:D:108:ARG:O	2.11	0.50
1:C:51:LEU:HD23	1:C:69:ILE:HG22	1.93	0.50
2:B:49:TYR:CG	3:E:513:VAL:HB	2.47	0.49
1:H:117:LYS:HG2	1:H:118:GLY:N	2.27	0.49
2:J:71:PHE:CD2	2:J:71:PHE:N	2.80	0.49
2:B:37:LEU:HB2	2:B:47:LEU:HD11	1.94	0.49
1:K:21:THR:HG23	1:K:77:GLN:HG2	1.94	0.49
1:K:82(A):THR:HG22	1:K:82(B):SER:OG	2.12	0.49
1:A:93:VAL:HG12	1:A:95:GLU:HG3	1.94	0.49
2:D:119:PRO:HG3	2:D:209:PHE:CG	2.48	0.49
1:H:64:GLU:OE1	1:K:105:ARG:NH2	2.46	0.48
2:J:83:VAL:HG13	2:J:103:LYS:NZ	2.28	0.48
1:A:2:VAL:HA	1:A:25:SER:O	2.13	0.48
2:B:11:LEU:C	2:B:11:LEU:HD23	2.39	0.48
1:K:20:LEU:HD12	1:K:80:LEU:HD23	1.95	0.48
1:C:52:TYR:CZ	1:C:53:ASN:HB2	2.48	0.48
1:C:162:GLY:O	1:C:182:VAL:HA	2.14	0.48
1:H:40:PRO:HB2	1:H:43:LYS:HB2	1.96	0.48
2:J:11:LEU:HD21	2:J:13:VAL:CG2	2.12	0.48
1:C:98:ILE:HD12	1:C:100:ALA:HB3	1.96	0.48
2:J:29:LEU:HD13	2:J:33:VAL:CG1	2.41	0.48
2:J:24:ARG:CZ	2:J:70:ASP:CG	2.87	0.48
1:C:66:ARG:NH2	1:C:82:LEU:HD11	2.29	0.47
2:D:49:TYR:CG	3:I:513:VAL:HB	2.48	0.47
2:D:159:SER:HA	2:D:178:THR:O	2.14	0.47
1:C:31(B):HIS:ND1	1:C:98:ILE:HD11	2.29	0.47
1:C:18:LEU:HD12	1:C:109:VAL:HG11	1.96	0.47
2:D:30(A):HIS:HB3	2:D:30(C):ASN:OD1	2.15	0.47
1:C:38:ARG:HB3	1:C:48:ILE:HD11	1.95	0.47
2:L:29:LEU:HA	2:L:92:LEU:HD22	1.97	0.47
1:C:168:ALA:HA	1:C:178:LEU:HB3	1.96	0.47
2:D:77:ARG:NH2	2:D:79:GLU:CD	2.72	0.47
2:J:33:VAL:CG2	2:J:51:VAL:HG22	2.45	0.47
2:B:4:MET:HE3	2:B:23:CYS:SG	2.55	0.46
2:J:158:ASN:HB3	2:J:180:THR:O	2.14	0.46
2:D:37:LEU:HB2	2:D:47:LEU:HD11	1.97	0.46
2:J:77:ARG:O	2:J:77:ARG:HG3	2.14	0.46
2:L:190:LYS:HZ1	2:L:210:ASN:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ALA:HA	1:A:178:LEU:HB3	1.97	0.46
2:B:155:LYS:C	2:B:155:LYS:HD3	2.41	0.46
2:B:24:ARG:NH2	2:B:70:ASP:CG	2.71	0.46
2:L:147:LYS:HD3	2:L:154:LEU:CD1	2.46	0.46
1:A:74:SER:OG	1:C:72:ASP:OD1	2.33	0.46
1:C:138:LEU:HD22	1:C:211:VAL:HG12	1.98	0.46
2:B:29:LEU:HA	2:B:92:LEU:HD22	1.98	0.46
1:H:74:SER:HB3	1:K:74:SER:OG	2.15	0.45
1:K:40:PRO:HB2	1:K:43:LYS:HD3	1.99	0.45
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.97	0.45
1:H:135:THR:HG22	1:H:185:PRO:HA	1.98	0.45
1:H:162:GLY:O	1:H:182:VAL:HA	2.17	0.45
2:J:77:ARG:NH2	2:D:74:LYS:HE2	2.32	0.45
2:B:55:ALA:O	2:B:58:VAL:HG12	2.16	0.45
2:J:130:VAL:HG21	2:J:186:TYR:HB2	1.98	0.45
1:K:155:ASN:O	1:K:158:SER:OG	2.33	0.45
1:A:143:LYS:HD2	1:A:143:LYS:HA	1.81	0.45
2:L:13:VAL:HG11	2:L:78:VAL:HG21	1.99	0.45
2:J:136:LEU:HD11	2:J:196:VAL:CG2	2.41	0.45
2:B:24:ARG:CZ	2:B:70:ASP:CG	2.90	0.44
2:J:67:SER:O	2:J:71:PHE:CE1	2.70	0.44
2:J:77:ARG:CZ	2:D:74:LYS:HE2	2.47	0.44
1:H:56:ARG:HG3	1:H:57:ILE:H	1.83	0.44
2:J:151:ASP:HA	2:J:191:VAL:HG12	1.98	0.44
2:J:67:SER:O	2:J:71:PHE:CZ	2.70	0.44
1:K:162:GLY:O	1:K:182:VAL:HA	2.17	0.44
1:K:192:GLN:HG2	1:K:194:TYR:CZ	2.53	0.44
2:L:34:HIS:CE1	3:F:512:ALA:HB1	2.53	0.44
1:C:60:ASN:O	1:C:64:GLU:N	2.49	0.44
1:C:122:PHE:CE1	2:D:123:ASP:OD2	2.71	0.44
1:H:56:ARG:HG3	1:K:25:SER:HB2	1.99	0.44
1:K:60:ASN:ND2	1:K:62:SER:OG	2.50	0.44
2:L:147:LYS:HD3	2:L:154:LEU:HD12	2.00	0.44
2:B:9:LEU:HD23	2:B:10:SER:OG	2.19	0.43
1:C:66:ARG:HD2	1:C:82(A):THR:O	2.18	0.43
1:K:22:CYS:HB3	1:K:78:PHE:HB3	1.99	0.43
1:H:52:TYR:HE2	1:H:97:VAL:HG11	1.82	0.43
1:A:168:ALA:HB2	1:A:178:LEU:HD23	1.99	0.43
2:B:24:ARG:CZ	2:B:70:ASP:HB2	2.45	0.43
2:J:124:GLN:OE1	2:J:131:SER:N	2.49	0.43
2:D:47:LEU:HA	2:D:58:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:ILE:O	1:H:29:ILE:HG13	2.19	0.43
2:L:39:LYS:HE2	2:L:81:GLU:O	2.19	0.43
2:B:13:VAL:HG11	2:B:78:VAL:CB	2.47	0.42
2:J:29:LEU:HD12	2:J:33:VAL:HG11	2.00	0.42
2:B:17:GLU:OE2	2:L:18:PRO:HD2	2.19	0.42
1:H:151:THR:OG1	1:H:199:ASN:HB3	2.19	0.42
1:C:119:PRO:HB3	1:C:145:TYR:HB3	2.00	0.42
2:D:34:HIS:O	2:D:88:CYS:HA	2.19	0.42
2:J:111:ALA:HA	2:D:143:GLU:OE2	2.19	0.42
2:B:113:PRO:HB3	2:B:139:PHE:HB3	2.02	0.42
1:C:66:ARG:CZ	1:C:82:LEU:HD11	2.49	0.42
2:B:18:PRO:HA	2:B:75:ILE:O	2.19	0.42
2:B:130:VAL:HG11	2:B:186:TYR:HB2	2.00	0.42
1:H:39:GLN:HB2	1:H:45:LEU:HD23	2.01	0.42
2:J:47:LEU:O	2:J:48:ILE:HD13	2.20	0.42
1:K:12:VAL:O	1:K:111:VAL:HA	2.19	0.42
2:L:18:PRO:HA	2:L:75:ILE:O	2.20	0.42
1:H:186:SER:HA	1:H:189:LEU:HG	2.01	0.41
1:K:151:THR:OG1	1:K:199:ASN:HB3	2.20	0.41
1:C:36:TRP:CG	1:C:80:LEU:HD13	2.55	0.41
2:D:24:ARG:NH2	2:D:70:ASP:CB	2.79	0.41
2:D:4:MET:HE3	2:D:23:CYS:SG	2.60	0.41
1:H:56:ARG:CG	1:H:57:ILE:N	2.83	0.41
2:L:28:SER:HA	2:L:69:THR:HG22	2.01	0.41
2:J:49:TYR:CG	3:G:513:VAL:HB	2.55	0.41
2:J:80:ALA:HA	2:J:106:ILE:HD11	2.02	0.41
1:K:210:ARG:NH1	1:K:212:GLU:CD	2.79	0.41
1:A:1:GLN:O	1:C:56:ARG:NH1	2.49	0.41
2:B:13:VAL:HG21	2:B:19:ALA:HB2	2.03	0.41
1:H:36:TRP:CE2	1:H:80:LEU:HB2	2.55	0.41
1:H:192:GLN:HG3	1:H:193:THR:N	2.34	0.41
2:L:37:LEU:HD23	2:L:86:TYR:CE1	2.55	0.41
2:B:54:ARG:NH1	2:B:60:ASP:OD1	2.49	0.41
1:K:71:LYS:HB3	1:K:71:LYS:HE3	1.70	0.40
1:C:29:ILE:HD12	1:C:34:TRP:CH2	2.56	0.40
1:A:146:PHE:HA	1:A:147:PRO:HA	1.83	0.40
1:C:64:GLU:HA	1:C:67:VAL:HG12	2.03	0.40
2:J:24:ARG:HH21	2:J:24:ARG:HD3	1.54	0.40
1:K:210:ARG:HH11	1:K:212:GLU:HB2	1.86	0.40
1:C:47:TRP:CH2	1:C:49:GLY:HA2	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ARG:NH2	2:D:81:GLU:OE1[1_556]	2.06	0.14
1:A:56:ARG:NH2	1:H:1:GLN:O[1_565]	2.18	0.02
1:K:56:ARG:NH2	1:C:1:GLN:O[1_545]	2.18	0.02

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	213/223 (96%)	210 (99%)	3 (1%)	0	100	100
1	C	215/223 (96%)	211 (98%)	4 (2%)	0	100	100
1	H	215/223 (96%)	212 (99%)	3 (1%)	0	100	100
1	K	215/223 (96%)	210 (98%)	5 (2%)	0	100	100
2	B	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
2	D	215/217 (99%)	211 (98%)	4 (2%)	0	100	100
2	J	148/217 (68%)	145 (98%)	3 (2%)	0	100	100
2	L	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
3	E	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
3	G	6/8 (75%)	6 (100%)	0	0	100	100
3	I	6/8 (75%)	6 (100%)	0	0	100	100
All	All	1675/1792 (94%)	1642 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	187/193 (97%)	187 (100%)	0	100	100
1	C	189/193 (98%)	185 (98%)	4 (2%)	47	66
1	H	189/193 (98%)	189 (100%)	0	100	100
1	K	189/193 (98%)	189 (100%)	0	100	100
2	B	192/192 (100%)	192 (100%)	0	100	100
2	D	192/192 (100%)	191 (100%)	1 (0%)	81	90
2	J	192/192 (100%)	187 (97%)	5 (3%)	40	59
2	L	192/192 (100%)	191 (100%)	1 (0%)	81	90
3	E	4/4 (100%)	4 (100%)	0	100	100
3	F	4/4 (100%)	4 (100%)	0	100	100
3	G	4/4 (100%)	4 (100%)	0	100	100
3	I	4/4 (100%)	4 (100%)	0	100	100
All	All	1538/1556 (99%)	1527 (99%)	11 (1%)	76	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	25	SER
2	J	31	THR
2	J	52	SER
2	J	65	SER
2	J	70	ASP
2	L	22	SER
1	C	132	SER
1	C	134	SER
1	C	135	THR
1	C	186	SER
2	D	76	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN

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Mol	Chain	Res	Type
2	B	93	GLN
1	H	1	GLN
1	H	31(B)	HIS
1	H	75	GLN
2	J	53	ASN
2	J	137	ASN
2	J	171	ASN
1	K	53	ASN
1	K	60	ASN
1	K	164	HIS
2	L	27	GLN
2	L	53	ASN
2	L	160	GLN
1	C	53	ASN
1	C	171	GLN
2	D	189	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	217/223 (97%)	0.17	7 (3%) 50 52	14, 22, 38, 59	0
1	C	219/223 (98%)	0.29	8 (3%) 45 48	15, 23, 43, 68	0
1	H	219/223 (98%)	0.41	10 (4%) 37 39	15, 24, 44, 62	0
1	K	219/223 (98%)	0.29	8 (3%) 45 48	13, 22, 44, 61	0
2	B	217/217 (100%)	0.23	7 (3%) 50 52	13, 23, 39, 55	0
2	D	217/217 (100%)	0.47	10 (4%) 37 39	15, 27, 44, 55	0
2	J	217/217 (100%)	0.62	20 (9%) 14 16	14, 30, 49, 55	0
2	L	217/217 (100%)	0.73	22 (10%) 12 14	15, 32, 53, 60	0
3	E	8/8 (100%)	0.37	0 100 100	17, 22, 27, 28	0
3	F	8/8 (100%)	0.77	0 100 100	26, 32, 36, 38	0
3	G	8/8 (100%)	1.13	0 100 100	32, 36, 43, 47	0
3	I	8/8 (100%)	0.74	0 100 100	25, 28, 35, 42	0
All	All	1774/1792 (98%)	0.41	92 (5%) 33 34	13, 25, 47, 68	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	41	GLY	4.4
2	J	78	VAL	4.0
2	D	123	ASP	3.9
2	B	17	GLU	3.9
1	H	213	ILE	3.5
1	C	126	PRO	3.4
1	A	213	ILE	3.3
1	C	132	SER	3.3
1	K	64	GLU	3.3
2	B	80	ALA	3.2
1	K	132	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	133	GLU	3.2
2	L	52	SER	3.1
1	K	56	ARG	3.1
1	H	100(B)	GLY	3.1
1	A	134	SER	3.0
2	L	123	ASP	3.0
2	J	60	ASP	3.0
1	C	99	ALA	2.9
1	H	74	SER	2.9
2	J	68	GLY	2.9
1	K	213	ILE	2.9
2	D	185	GLU	2.8
2	L	56	SER	2.8
2	L	51	VAL	2.8
2	J	23	CYS	2.8
2	J	126	LYS	2.8
1	C	42	GLY	2.7
2	J	57	GLY	2.7
2	J	54	ARG	2.7
2	J	11	LEU	2.7
1	C	213	ILE	2.7
2	L	59	PRO	2.7
1	K	63	LEU	2.7
1	A	44	GLY	2.6
1	H	132	SER	2.6
2	L	30(B)	SER	2.6
1	A	1	GLN	2.6
1	H	126	PRO	2.6
1	A	188	SER	2.6
1	H	100(C)	THR	2.5
2	J	92	LEU	2.5
2	J	154	LEU	2.5
2	L	74	LYS	2.5
2	L	212	GLY	2.5
1	K	98	ILE	2.4
2	L	70	ASP	2.4
2	J	24	ARG	2.4
2	L	65	SER	2.4
2	B	212	GLY	2.4
2	L	14	THR	2.4
2	L	16	GLY	2.3
2	D	57	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	57	GLY	2.3
2	L	31	THR	2.3
2	B	15	PRO	2.3
1	H	188	SER	2.3
2	D	212	GLY	2.3
1	A	135	THR	2.3
1	A	127	SER	2.3
2	L	76	SER	2.3
2	L	61	ARG	2.2
1	K	99	ALA	2.2
2	B	13	VAL	2.2
2	J	58	VAL	2.2
1	K	31(A)	SER	2.2
2	J	67	SER	2.2
2	L	67	SER	2.2
1	H	56	ARG	2.2
2	D	30	LEU	2.2
2	J	123	ASP	2.2
2	J	79	GLU	2.2
2	B	14	THR	2.2
2	D	77	ARG	2.1
2	B	78	VAL	2.1
2	J	16	GLY	2.1
2	D	153	ALA	2.1
1	C	9	PRO	2.1
2	D	78	VAL	2.1
1	C	44	GLY	2.1
2	D	54	ARG	2.1
2	J	122	GLU	2.1
2	J	15	PRO	2.1
2	J	185	GLU	2.1
2	L	78	VAL	2.1
2	L	68	GLY	2.1
1	C	43	LYS	2.0
2	J	63	SER	2.0
2	D	56	SER	2.0
2	L	189	HIS	2.0
1	H	189	LEU	2.0
2	L	60	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.