



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:13 PM UTC

PDB ID : 2WZP / pdb_00002wzp
Title : Structures of Lactococcal Phage p2 Baseplate Shed Light on a Novel Mechanism of Host Attachment and Activation in Siphoviridae
Authors : Sciara, G.; Bebeacua, C.; Bron, P.; Tremblay, D.; Ortiz-Lombardia, M.; Lichiere, J.; van Heel, M.; Campanacci, V.; Moineau, S.; Cambillau, C.
Deposited on : 2009-12-01
Resolution : 2.60 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

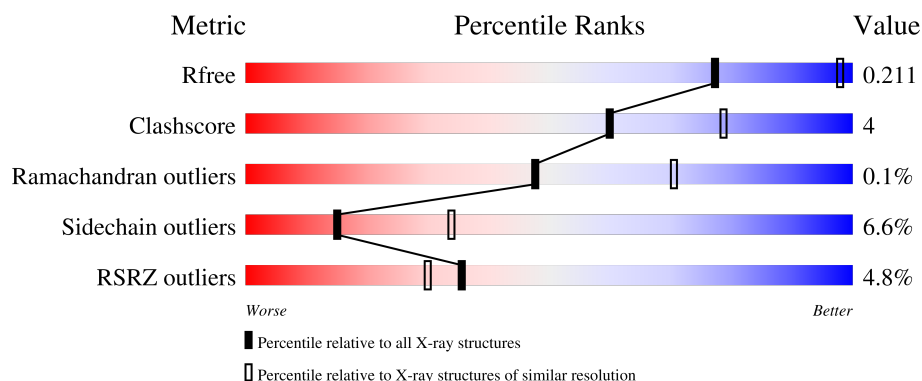
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



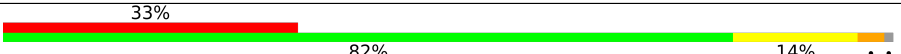
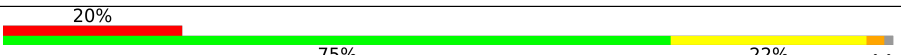
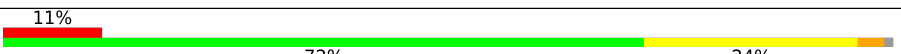
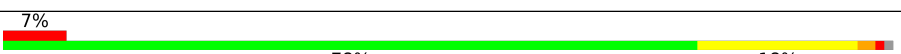
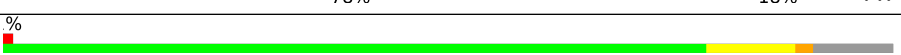
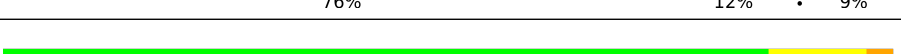
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	266	4% 90% 9%
1	B	266	89% 10%
1	C	266	3% 89% 10%
1	G	266	% 85% 14%
1	H	266	2% 88% 9%

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Mol	Chain	Length	Quality of chain
1	I	266	
2	D	123	
2	E	123	
2	F	123	
2	J	123	
2	K	123	
2	L	123	
3	P	326	
3	Q	326	
4	R	375	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27647 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 PUTATIVE RECEPTOR BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2024	1269	349	400	6			
1	B	266	Total	C	N	O	S	0	0	0
			2024	1269	349	400	6			
1	C	266	Total	C	N	O	S	0	0	0
			2024	1269	349	400	6			
1	G	266	Total	C	N	O	S	0	0	0
			2024	1269	349	400	6			
1	H	266	Total	C	N	O	S	0	0	0
			2024	1269	349	400	6			
1	I	266	Total	C	N	O	S	0	0	0
			2024	1269	349	400	6			

- Molecule 2 is a protein called CAMELID VHH5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	122	Total	C	N	O	S	0	0	0
			938	581	165	186	6			
2	E	122	Total	C	N	O	S	0	0	0
			922	572	158	186	6			
2	F	122	Total	C	N	O	S	0	0	0
			931	575	165	185	6			
2	J	122	Total	C	N	O	S	0	0	0
			938	581	165	186	6			
2	K	122	Total	C	N	O	S	0	0	0
			938	581	165	186	6			
2	L	122	Total	C	N	O	S	0	0	0
			938	581	165	186	6			

- Molecule 3 is a protein called LACTOCOCCAL PHAGE P2 ORF15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	Q	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			

- Molecule 4 is a protein called LACTOCOCCAL PHAGE P2 ORF16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	375	Total	C	N	O	S	0	0	0
			3025	1934	497	586	8			

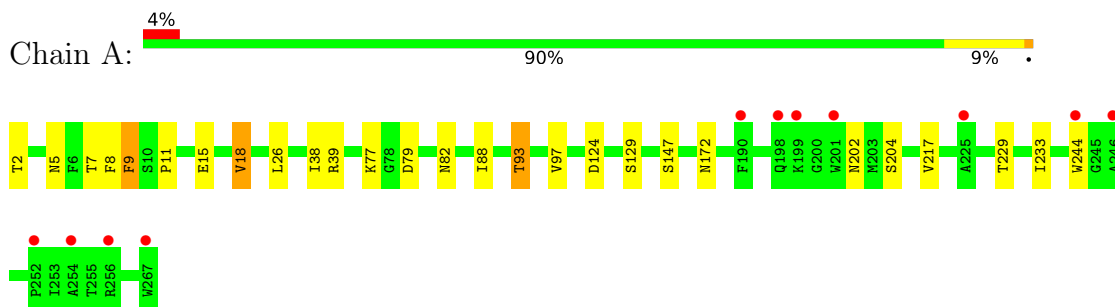
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	B	85	Total	O	0	0
			85	85		
5	C	112	Total	O	0	0
			112	112		
5	D	11	Total	O	0	0
			11	11		
5	E	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		
5	G	199	Total	O	0	0
			199	199		
5	H	156	Total	O	0	0
			156	156		
5	I	192	Total	O	0	0
			192	192		
5	K	3	Total	O	0	0
			3	3		
5	L	7	Total	O	0	0
			7	7		
5	P	363	Total	O	0	0
			363	363		
5	Q	265	Total	O	0	0
			265	265		
5	R	567	Total	O	0	0
			567	567		

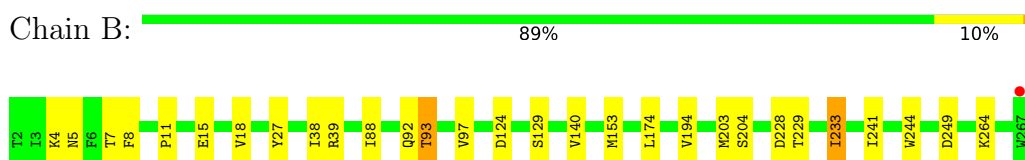
3 Residue-property plots [i](#)

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.

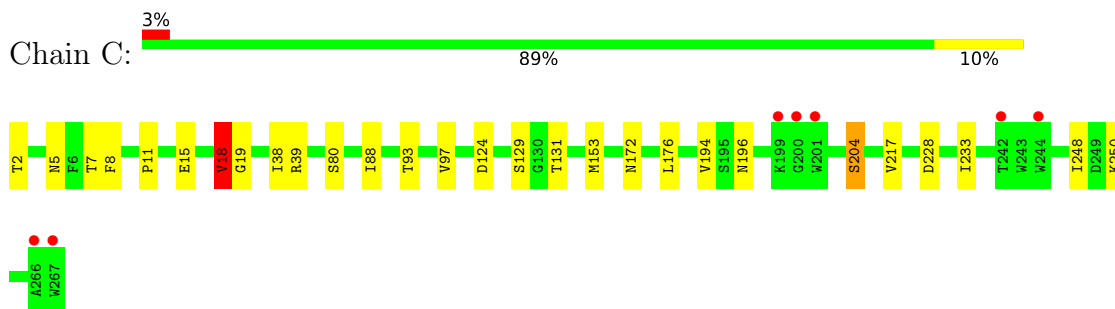
- Molecule 1: PUTATIVE RECEPTOR BINDING PROTEIN



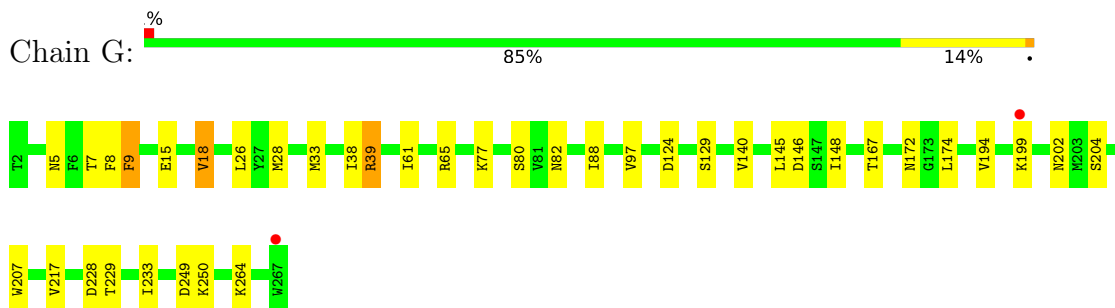
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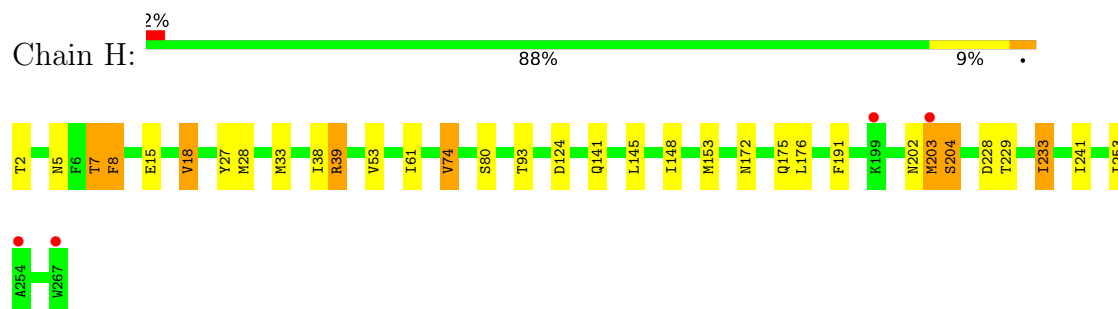
- Molecule 1: PUTATIVE RECEPTOR BINDING PROTEIN



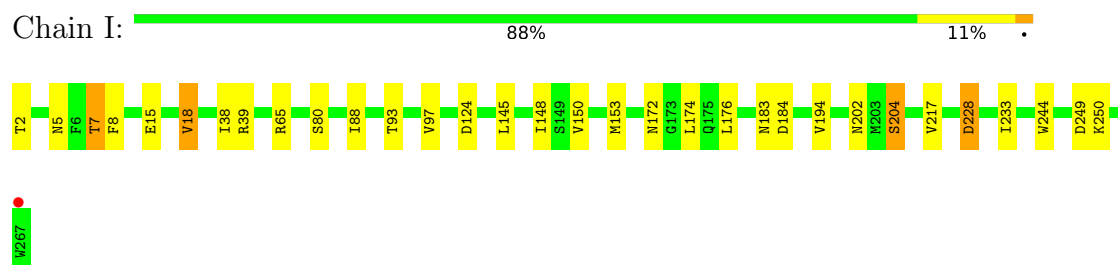
- Molecule 1: PUTATIVE RECEPTOR BINDING PROTEIN



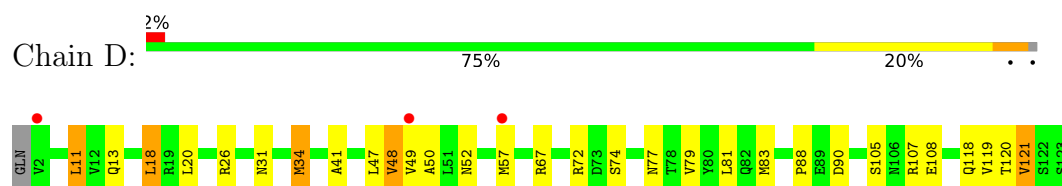
- Molecule 1: PUTATIVE RECEPTOR BINDING PROTEIN



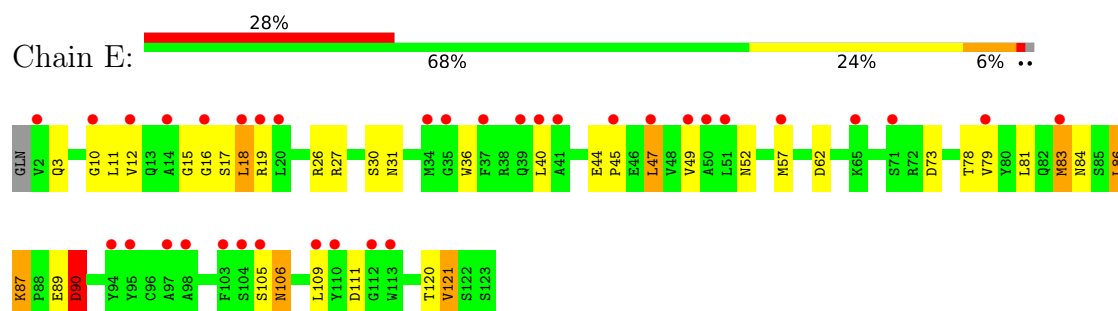
- Molecule 1: PUTATIVE RECEPTOR BINDING PROTEIN



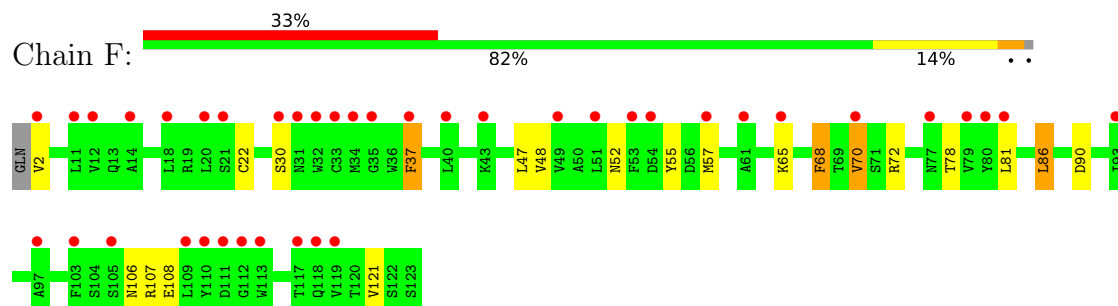
- Molecule 2: CAMELID VHH5



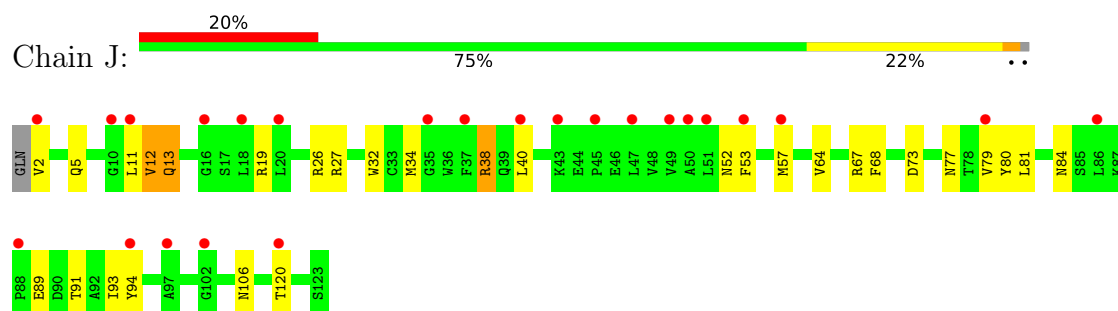
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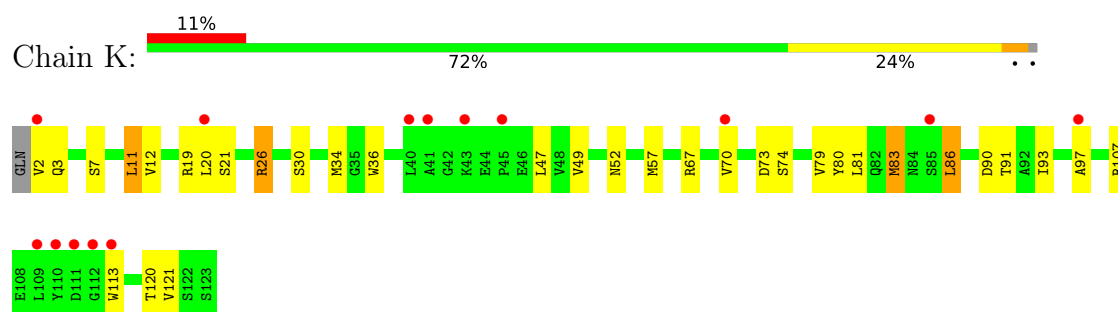
- Molecule 2: CAMELID VHH5



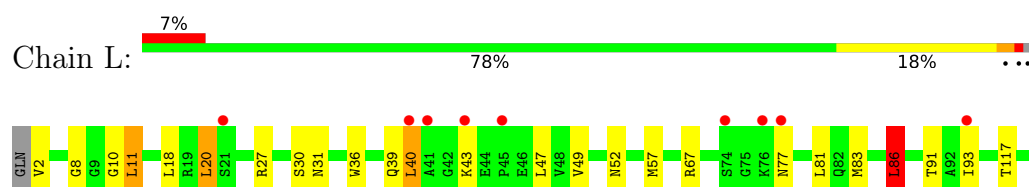
- Molecule 2: CAMELID VHH5



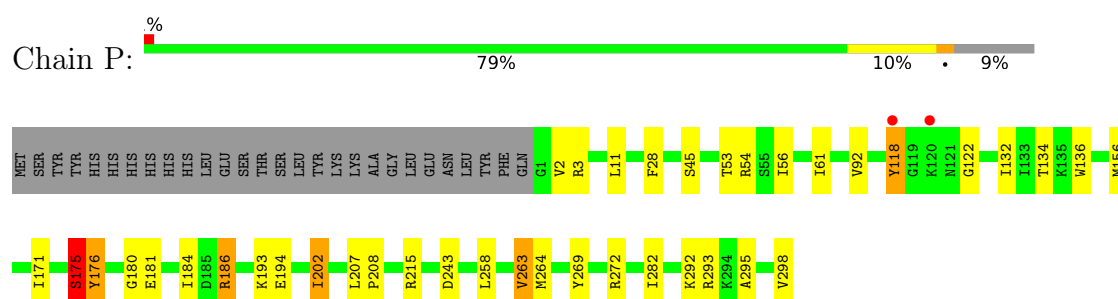
- Molecule 2: CAMELID VHH5



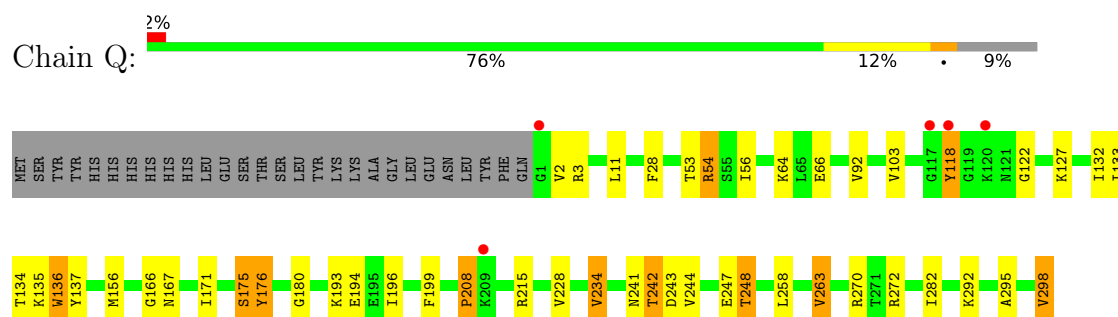
- Molecule 2: CAMELID VHH5



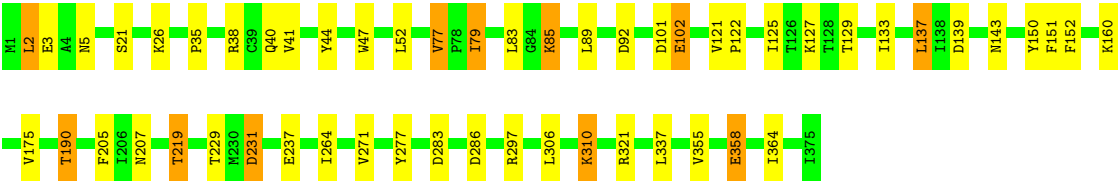
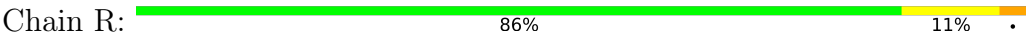
- Molecule 3: LACTOCOCCAL PHAGE P2 ORF15



- Molecule 3: LACTOCOCCAL PHAGE P2 ORF15



● Molecule 4: LACTOCOCCAL PHAGE P2 ORF16



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	202.88Å 202.88Å 760.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.07 – 2.60 38.07 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.07-2.60) 99.3 (38.07-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.179 , 0.208 0.184 , 0.211	Depositor DCC
R_{free} test set	3689 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27647	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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	0.62	0/2064	1.00	4/2813 (0.1%)
1	B	0.62	0/2064	1.04	8/2813 (0.3%)
1	C	0.63	0/2064	1.00	5/2813 (0.2%)
1	G	0.69	0/2064	1.09	7/2813 (0.2%)
1	H	0.68	1/2064 (0.0%)	1.10	7/2813 (0.2%)
1	I	0.69	0/2064	1.07	8/2813 (0.3%)
2	D	0.69	1/956 (0.1%)	1.13	1/1289 (0.1%)
2	E	0.76	0/940	1.30	7/1271 (0.6%)
2	F	0.79	0/948	1.24	5/1278 (0.4%)
2	J	0.80	0/956	1.23	2/1289 (0.2%)
2	K	0.75	0/956	1.21	2/1289 (0.2%)
2	L	0.75	0/956	1.18	2/1289 (0.2%)
3	P	0.81	1/2485 (0.0%)	1.23	10/3356 (0.3%)
3	Q	0.79	0/2485	1.25	11/3356 (0.3%)
4	R	0.90	1/3094 (0.0%)	1.29	10/4208 (0.2%)
All	All	0.74	4/26160 (0.0%)	1.16	89/35503 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	175	SER	CA-C	-5.72	1.45	1.52
1	H	203	MET	SD-CE	-5.58	1.65	1.79
2	D	34	MET	SD-CE	-5.42	1.66	1.79
4	R	77	VAL	CA-C	5.32	1.58	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	208	PRO	N-CA-C	9.07	126.44	113.47
4	R	85	LYS	N-CA-C	7.90	121.26	108.63
3	P	118	TYR	N-CA-C	7.07	120.47	110.23
1	B	15	GLU	N-CA-C	7.00	118.56	111.07
3	Q	133	ILE	N-CA-C	-6.93	104.97	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	219	THR	CB-CA-C	6.73	120.85	109.75
2	J	106	ASN	CA-C-N	6.63	129.06	120.44
2	J	106	ASN	C-N-CA	6.63	129.06	120.44
3	Q	243	ASP	CA-CB-CG	6.63	119.23	112.60
3	Q	118	TYR	N-CA-C	6.52	119.93	110.28
1	C	129	SER	N-CA-C	-6.33	100.19	109.63
4	R	127	LYS	N-CA-C	6.30	118.95	111.71
3	Q	263	VAL	N-CA-CB	-6.24	104.22	112.26
1	C	15	GLU	N-CA-C	6.21	118.60	111.02
1	H	15	GLU	N-CA-C	6.19	117.90	111.03
4	R	358	GLU	CB-CG-CD	6.14	123.03	112.60
1	I	15	GLU	N-CA-C	6.13	118.50	111.02
1	G	18	VAL	N-CA-CB	6.05	118.29	111.21
1	A	15	GLU	N-CA-C	6.03	118.34	111.11
3	P	2	VAL	CA-C-N	5.98	129.78	120.75
3	P	2	VAL	C-N-CA	5.98	129.78	120.75
3	Q	263	VAL	CB-CA-C	5.91	118.53	111.20
4	R	129	THR	N-CA-C	5.91	118.33	110.53
3	P	263	VAL	CB-CA-C	5.90	119.34	111.85
4	R	286	ASP	CA-CB-CG	5.86	118.46	112.60
2	E	17	SER	N-CA-C	5.83	118.78	110.10
1	G	15	GLU	N-CA-C	5.79	117.27	111.07
2	E	17	SER	CA-C-N	5.76	132.05	121.85
2	E	17	SER	C-N-CA	5.76	132.05	121.85
1	G	39	ARG	N-CA-C	-5.71	99.59	108.90
1	B	129	SER	N-CA-C	-5.70	100.11	109.80
1	G	249	ASP	CA-C-N	5.66	128.43	120.28
1	G	249	ASP	C-N-CA	5.66	128.43	120.28
2	E	90	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	129	SER	N-CA-C	-5.62	100.25	109.80
3	Q	28	PHE	CA-CB-CG	5.59	119.39	113.80
2	F	37	PHE	CA-CB-CG	5.55	119.35	113.80
2	F	90	ASP	N-CA-C	-5.53	106.20	113.17
1	I	204	SER	N-CA-C	5.52	119.64	113.01
1	B	92	GLN	CA-C-N	5.51	127.92	120.38
1	B	92	GLN	C-N-CA	5.51	127.92	120.38
4	R	101	ASP	CA-CB-CG	5.51	118.11	112.60
1	I	18	VAL	N-CA-CB	5.48	118.25	111.41
3	P	28	PHE	CA-CB-CG	5.47	119.28	113.80
1	H	39	ARG	N-CA-C	-5.47	99.98	108.90
1	G	228	ASP	CA-CB-CG	5.46	118.06	112.60
1	H	18	VAL	CB-CA-C	5.46	118.46	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	VAL	N-CA-CB	5.46	118.23	111.41
1	H	204	SER	N-CA-C	5.44	119.66	113.19
2	L	10	GLY	N-CA-C	5.43	117.05	111.56
2	D	48	VAL	CB-CA-C	5.43	115.84	111.06
2	K	74	SER	CA-C-N	5.43	126.97	120.13
2	K	74	SER	C-N-CA	5.43	126.97	120.13
3	P	272	ARG	N-CA-C	-5.41	106.69	113.72
1	B	249	ASP	CA-C-N	5.37	128.01	120.28
1	B	249	ASP	C-N-CA	5.37	128.01	120.28
1	I	228	ASP	CA-CB-CG	5.33	117.94	112.60
2	E	18	LEU	N-CA-C	-5.33	100.62	108.99
2	E	10	GLY	N-CA-C	5.32	116.74	111.21
1	C	18	VAL	N-CA-CB	5.31	118.05	111.41
3	P	263	VAL	N-CA-CB	-5.30	105.23	112.28
1	H	8	PHE	CA-C-N	5.30	128.29	120.82
1	H	8	PHE	C-N-CA	5.30	128.29	120.82
3	Q	2	VAL	CA-C-N	5.28	128.72	120.75
3	Q	2	VAL	C-N-CA	5.28	128.72	120.75
3	Q	64	LYS	N-CA-C	-5.26	100.59	108.96
3	P	243	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	204	SER	N-CA-C	5.25	119.43	113.19
4	R	79	ILE	CA-CB-CG2	5.22	119.38	110.50
4	R	92	ASP	CA-CB-CG	5.19	117.79	112.60
1	H	93	THR	N-CA-C	5.18	117.60	111.33
4	R	231	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	39	ARG	N-CA-C	-5.17	100.97	109.40
2	F	107	ARG	CA-C-N	5.17	127.92	120.38
2	F	107	ARG	C-N-CA	5.17	127.92	120.38
1	I	184	ASP	CA-CB-CG	5.16	117.76	112.60
1	I	249	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	39	ARG	N-CA-C	-5.13	100.53	108.90
1	I	39	ARG	N-CA-C	-5.11	100.57	108.90
1	G	129	SER	N-CA-C	-5.09	102.04	109.63
2	L	86	LEU	N-CA-C	5.09	117.07	109.59
2	F	68	PHE	CA-CB-CG	5.08	118.89	113.80
1	I	93	THR	N-CA-C	5.08	117.48	111.33
2	E	106	ASN	CA-CB-CG	5.05	117.65	112.60
3	Q	234	VAL	N-CA-CB	5.04	116.51	110.31
1	B	204	SER	N-CA-C	5.04	119.19	113.19
1	A	39	ARG	N-CA-C	-5.03	100.71	108.90
3	P	184	ILE	CA-C-N	5.01	127.50	120.28
3	P	184	ILE	C-N-CA	5.01	127.50	120.28

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	2024	0	1983	18	0
1	B	2024	0	1983	20	0
1	C	2024	0	1983	17	0
1	G	2024	0	1983	19	0
1	H	2024	0	1983	18	0
1	I	2024	0	1983	12	0
2	D	938	0	891	15	0
2	E	922	0	858	18	0
2	F	931	0	884	8	0
2	J	938	0	891	12	0
2	K	938	0	891	16	0
2	L	938	0	891	12	0
3	P	2432	0	2394	19	0
3	Q	2432	0	2394	27	0
4	R	3025	0	2984	23	0
5	A	47	0	0	0	0
5	B	85	0	0	1	0
5	C	112	0	0	0	0
5	D	11	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	199	0	0	2	0
5	H	156	0	0	0	0
5	I	192	0	0	0	0
5	K	3	0	0	0	0
5	L	7	0	0	0	0
5	P	363	0	0	0	0
5	Q	265	0	0	1	0
5	R	567	0	0	3	0
All	All	27647	0	24976	218	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 4.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:THR:HG23	1:C:11:PRO:HG2	1.28	1.08
1:A:93:THR:CG2	1:C:11:PRO:HG2	2.06	0.86
1:A:93:THR:HG23	1:C:11:PRO:CG	2.09	0.83
1:A:77:LYS:H	1:A:82:ASN:HD21	1.31	0.77
1:C:194:VAL:HG13	1:C:248:ILE:HD12	1.68	0.76
2:E:15:GLY:HA2	2:E:86:LEU:HB2	1.67	0.76
1:B:203:MET:HE1	1:B:233:ILE:CG2	2.16	0.75
3:P:156:MET:O	3:P:176:TYR:HA	1.86	0.75
1:H:153:MET:HE1	1:I:153:MET:HE1	1.69	0.75
3:Q:156:MET:O	3:Q:176:TYR:HA	1.86	0.74
1:A:244:TRP:HE1	2:E:31:ASN:HD21	1.36	0.72
3:P:136:TRP:HB2	3:P:295:ALA:O	1.90	0.71
2:J:32:TRP:HE1	2:J:34:MET:HE3	1.54	0.71
2:F:52:ASN:HD22	2:F:55:TYR:HB2	1.53	0.71
1:C:194:VAL:HG13	1:C:248:ILE:CD1	2.21	0.70
3:Q:171:ILE:H	3:Q:175:SER:HA	1.57	0.68
1:B:203:MET:HE1	1:B:233:ILE:HG22	1.73	0.68
2:D:20:LEU:HD12	2:D:81:LEU:HD23	1.76	0.68
3:Q:199:PHE:H	3:Q:242:THR:HG22	1.58	0.67
2:J:27:ARG:HD2	2:J:77:ASN:HD21	1.60	0.67
1:B:244:TRP:HE1	2:D:31:ASN:HD21	1.40	0.66
4:R:102:GLU:CD	4:R:102:GLU:H	1.99	0.66
1:H:203:MET:HE3	1:H:241:ILE:HG22	1.76	0.66
3:P:175:SER:OG	3:P:176:TYR:N	2.21	0.66
1:H:203:MET:HE1	1:H:233:ILE:CG2	2.26	0.66
2:K:7:SER:HB3	2:K:21:SER:HB3	1.77	0.65
3:Q:208:PRO:HA	3:Q:234:VAL:HG22	1.79	0.65
1:B:203:MET:HE3	1:B:241:ILE:HG22	1.77	0.65
3:Q:136:TRP:HB2	3:Q:295:ALA:O	1.97	0.64
4:R:237:GLU:CD	4:R:321:ARG:HH22	2.05	0.64
1:A:11:PRO:HG2	1:B:93:THR:HG23	1.80	0.63
2:J:64:VAL:HB	2:J:68:PHE:CD1	2.33	0.63
2:L:18:LEU:HB3	2:L:83:MET:HE3	1.79	0.63
1:H:53:VAL:HG13	1:H:74:VAL:HG13	1.78	0.63
5:G:2030:HOH:O	3:P:175:SER:HB2	1.98	0.63
1:G:77:LYS:H	1:G:82:ASN:HD21	1.47	0.62
3:Q:118:TYR:HB3	3:Q:122:GLY:HA2	1.82	0.62
2:J:73:ASP:HB2	2:J:80:TYR:CE2	2.35	0.62
3:Q:272:ARG:HD2	4:R:3:GLU:OE1	1.99	0.62
1:H:175:GLN:HE21	1:H:191:PHE:HB2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:171:ILE:H	3:P:175:SER:HA	1.64	0.61
1:G:264:LYS:NZ	5:G:2199:HOH:O	2.32	0.61
3:Q:175:SER:OG	3:Q:176:TYR:N	2.23	0.61
2:E:47:LEU:HD13	2:E:47:LEU:H	1.66	0.61
2:J:38:ARG:HB2	2:J:94:TYR:CE1	2.36	0.61
1:B:203:MET:HE1	1:B:233:ILE:HG21	1.84	0.60
1:C:131:THR:HA	3:P:202:ILE:HG13	1.84	0.59
2:L:49:VAL:HG21	2:L:81:LEU:HD13	1.84	0.59
4:R:358:GLU:HG3	5:R:2086:HOH:O	2.02	0.59
2:F:52:ASN:ND2	2:F:55:TYR:HB2	2.17	0.59
2:E:18:LEU:O	2:E:83:MET:HE1	2.02	0.59
1:B:203:MET:CE	1:B:233:ILE:HG22	2.34	0.58
2:K:73:ASP:HB2	2:K:80:TYR:CE2	2.39	0.58
1:A:172:ASN:HD21	1:A:204:SER:H	1.52	0.58
2:J:73:ASP:HB2	2:J:80:TYR:HE2	1.69	0.58
1:C:19:GLY:HA2	3:Q:166:GLY:O	2.03	0.57
4:R:150:TYR:CD1	4:R:152:PHE:HE1	2.22	0.57
4:R:122:PRO:HD2	4:R:125:ILE:HD12	1.87	0.57
1:H:203:MET:HE1	1:H:233:ILE:HG21	1.87	0.56
1:C:196:ASN:HD21	1:C:250:LYS:HG2	1.69	0.56
1:I:172:ASN:HD21	1:I:204:SER:H	1.52	0.56
2:D:47:LEU:HD21	2:D:50:ALA:HB2	1.87	0.55
2:E:36:TRP:CH2	2:E:79:VAL:HG12	2.42	0.55
1:H:203:MET:HE1	1:H:233:ILE:HG22	1.88	0.55
2:K:2:VAL:HG11	2:K:26:ARG:HG2	1.89	0.55
2:K:91:THR:HG23	2:K:120:THR:HA	1.89	0.54
1:G:172:ASN:HD21	1:G:204:SER:H	1.55	0.54
1:H:229:THR:HB	1:I:228:ASP:HB2	1.88	0.54
2:J:12:VAL:HG22	2:J:13:GLN:HE21	1.72	0.54
1:A:5:ASN:HB3	1:A:8:PHE:CD1	2.43	0.54
3:Q:3:ARG:C	3:Q:3:ARG:HD2	2.33	0.54
2:J:34:MET:HB2	2:J:53:PHE:CE1	2.43	0.54
1:I:244:TRP:HE1	2:L:31:ASN:HD21	1.54	0.53
2:E:87:LYS:HG3	2:E:89:GLU:H	1.74	0.53
2:E:11:LEU:HD12	2:E:120:THR:HB	1.91	0.52
3:P:194:GLU:HG3	3:P:293:ARG:NH1	2.24	0.52
1:C:88:ILE:HG12	1:C:97:VAL:HG22	1.90	0.52
1:A:217:VAL:HB	2:E:30:SER:CB	2.40	0.52
1:G:88:ILE:HG12	1:G:97:VAL:HG22	1.91	0.52
3:Q:132:ILE:HG23	3:Q:135:LYS:HB2	1.92	0.52
4:R:47:TRP:CZ3	4:R:364:ILE:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LYS:H	1:A:82:ASN:ND2	2.06	0.51
1:G:229:THR:HB	1:H:228:ASP:HB2	1.93	0.51
2:L:8:GLY:O	2:L:117:THR:HG21	2.09	0.51
2:L:67:ARG:HH21	2:L:86:LEU:HA	1.75	0.51
2:K:20:LEU:HD12	2:K:81:LEU:HD23	1.91	0.51
2:L:20:LEU:HD12	2:L:81:LEU:HB3	1.92	0.51
1:C:18:VAL:O	3:Q:167:ASN:HA	2.11	0.51
1:B:153:MET:HE1	1:C:153:MET:HE1	1.93	0.51
2:K:2:VAL:HG22	2:K:3:GLN:H	1.75	0.51
3:Q:103:VAL:HG21	3:Q:298:VAL:HG11	1.93	0.51
2:D:34:MET:HE1	2:D:77:ASN:HB3	1.93	0.50
1:A:9:PHE:HB2	3:Q:180:GLY:HA2	1.94	0.50
1:H:172:ASN:HD21	1:H:204:SER:H	1.57	0.50
3:Q:171:ILE:H	3:Q:175:SER:CA	2.23	0.50
4:R:277:TYR:OH	4:R:283:ASP:OD1	2.30	0.49
3:P:118:TYR:HB3	3:P:122:GLY:HA2	1.94	0.49
4:R:190:THR:HB	4:R:207:ASN:HD21	1.77	0.49
2:F:68:PHE:HB3	2:F:81:LEU:HD11	1.94	0.49
2:D:118:GLN:HE22	1:G:167:THR:H	1.60	0.49
1:G:5:ASN:HB3	1:G:8:PHE:CD1	2.47	0.49
1:A:172:ASN:ND2	1:A:204:SER:H	2.10	0.49
1:A:229:THR:HB	1:B:228:ASP:HB2	1.93	0.49
1:C:172:ASN:ND2	1:C:204:SER:H	2.11	0.49
2:L:91:THR:HG23	2:L:120:THR:HA	1.95	0.49
2:K:67:ARG:NH2	2:K:90:ASP:OD2	2.46	0.48
3:P:3:ARG:HD2	3:P:3:ARG:C	2.38	0.48
3:Q:134:THR:HG22	3:Q:137:TYR:CD2	2.48	0.48
1:B:5:ASN:HB3	1:B:8:PHE:CD1	2.48	0.48
2:L:40:LEU:O	2:L:43:LYS:HB3	2.13	0.48
3:Q:241:ASN:HD22	3:Q:242:THR:N	2.11	0.48
2:D:18:LEU:HB3	2:D:83:MET:HE3	1.96	0.48
2:F:22:CYS:O	2:F:78:THR:HA	2.13	0.48
2:K:73:ASP:HB2	2:K:80:TYR:HE2	1.78	0.48
2:E:49:VAL:HG21	2:E:81:LEU:HD13	1.95	0.48
1:I:5:ASN:HB3	1:I:8:PHE:CD1	2.48	0.48
1:I:88:ILE:HG12	1:I:97:VAL:HG22	1.96	0.48
2:E:47:LEU:HD13	2:E:47:LEU:N	2.28	0.48
1:B:203:MET:CE	1:B:233:ILE:CG2	2.89	0.48
1:A:88:ILE:HG12	1:A:97:VAL:HG22	1.95	0.48
2:E:44:GLU:HB3	2:E:45:PRO:HD2	1.96	0.48
1:G:146:ASP:HB3	1:H:141:GLN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:86:LEU:HD22	2:F:121:VAL:HG21	1.95	0.47
3:Q:136:TRP:HA	3:Q:136:TRP:CE3	2.48	0.47
1:H:5:ASN:HB3	1:H:8:PHE:CD1	2.50	0.47
2:K:2:VAL:HG11	2:K:26:ARG:CG	2.44	0.47
1:H:203:MET:CE	1:H:233:ILE:HG22	2.45	0.47
1:B:11:PRO:HG3	1:C:93:THR:HB	1.97	0.46
2:D:41:ALA:HA	1:G:207:TRP:CD1	2.50	0.46
2:D:83:MET:HE1	2:D:119:VAL:HG21	1.98	0.46
4:R:133:ILE:HG22	4:R:137:LEU:HD22	1.98	0.46
3:Q:244:VAL:HG12	3:Q:272:ARG:HD3	1.96	0.46
1:G:9:PHE:HB2	3:P:180:GLY:HA2	1.97	0.46
2:K:11:LEU:HG	2:K:120:THR:HB	1.98	0.46
3:Q:215:ARG:HB3	3:Q:282:ILE:HD11	1.97	0.46
4:R:139:ASP:H	4:R:143:ASN:ND2	2.13	0.46
2:F:70:VAL:HG13	2:F:81:LEU:HD13	1.98	0.46
3:P:171:ILE:H	3:P:175:SER:CA	2.27	0.46
1:A:11:PRO:HG2	1:B:93:THR:CG2	2.45	0.46
1:I:174:LEU:HB2	1:I:194:VAL:HG22	1.98	0.46
4:R:47:TRP:CE3	4:R:355:VAL:HB	2.50	0.46
1:B:244:TRP:NE1	2:D:31:ASN:HD21	2.13	0.45
2:E:86:LEU:HD12	2:E:121:VAL:HG22	1.98	0.45
3:Q:136:TRP:HA	3:Q:136:TRP:HE3	1.80	0.45
2:F:106:ASN:OD1	2:F:108:GLU:HB3	2.16	0.45
4:R:151:PHE:HE2	4:R:205:PHE:CD1	2.34	0.45
1:B:229:THR:HB	1:C:228:ASP:HB2	1.99	0.45
4:R:190:THR:HB	4:R:207:ASN:ND2	2.31	0.45
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.49	0.45
2:K:97:ALA:HB2	2:K:113:TRP:CZ3	2.51	0.45
1:I:217:VAL:HB	2:L:30:SER:CB	2.47	0.45
4:R:150:TYR:HD1	4:R:152:PHE:HE1	1.64	0.45
4:R:297:ARG:NH1	5:R:2475:HOH:O	2.50	0.45
1:A:26:LEU:HD21	1:B:27:TYR:CZ	2.52	0.45
2:D:72:ARG:NH2	2:D:74:SER:O	2.50	0.45
4:R:3:GLU:OE2	4:R:38:ARG:HD2	2.17	0.45
2:J:34:MET:HE1	2:J:77:ASN:O	2.17	0.45
2:J:67:ARG:HG2	2:J:84:ASN:O	2.18	0.44
1:A:147:SER:HB2	1:B:140:VAL:HG21	2.00	0.44
3:Q:134:THR:HG21	3:Q:292:LYS:HE2	2.00	0.44
1:G:174:LEU:HB2	1:G:194:VAL:HG22	1.99	0.44
1:G:217:VAL:HB	2:K:30:SER:CB	2.48	0.44
1:C:217:VAL:HB	2:F:30:SER:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:83:MET:HG3	2:K:86:LEU:HD11	2.00	0.43
2:E:86:LEU:HD13	2:E:90:ASP:HB2	2.00	0.43
3:P:61:ILE:HG13	3:P:132:ILE:HD11	2.01	0.43
1:B:88:ILE:HG12	1:B:97:VAL:HG22	2.00	0.43
4:R:297:ARG:NH2	5:R:2477:HOH:O	2.41	0.43
1:G:65:ARG:HD2	1:I:7:THR:O	2.19	0.43
2:J:91:THR:HG23	2:J:120:THR:HA	2.00	0.43
4:R:47:TRP:CZ3	4:R:355:VAL:HB	2.53	0.43
1:C:172:ASN:HD21	1:C:204:SER:H	1.65	0.43
2:E:47:LEU:HD12	2:E:105:SER:HA	2.01	0.43
2:L:27:ARG:HG3	2:L:77:ASN:HD21	1.84	0.43
2:E:16:GLY:HA2	2:E:84:ASN:HD22	1.84	0.43
2:L:11:LEU:HA	2:L:120:THR:O	2.18	0.43
1:G:77:LYS:H	1:G:82:ASN:ND2	2.13	0.43
1:G:39:ARG:HB2	1:G:61:ILE:HB	2.00	0.42
3:P:136:TRP:HA	3:P:136:TRP:CE3	2.54	0.42
3:Q:241:ASN:HB3	3:Q:248:THR:HG23	2.00	0.42
3:P:264:MET:SD	3:P:269:TYR:CD2	3.13	0.42
4:R:5:ASN:HB3	4:R:35:PRO:HG3	2.01	0.42
2:K:49:VAL:HG11	2:K:81:LEU:HD13	2.01	0.42
2:L:36:TRP:CZ3	2:L:81:LEU:HB2	2.54	0.42
2:K:36:TRP:CZ3	2:K:81:LEU:HB2	2.54	0.42
2:J:34:MET:HB2	2:J:53:PHE:HE1	1.83	0.42
2:D:11:LEU:HG	2:D:120:THR:HB	2.01	0.42
2:D:34:MET:HB3	2:D:79:VAL:HG11	2.02	0.42
1:H:39:ARG:HB2	1:H:61:ILE:HB	2.01	0.42
3:P:207:LEU:HA	3:P:208:PRO:HD3	1.95	0.42
4:R:271:VAL:HB	4:R:310:LYS:HG2	2.02	0.41
4:R:264:ILE:O	4:R:271:VAL:HA	2.19	0.41
4:R:2:LEU:HD22	4:R:44:TYR:CZ	2.55	0.41
1:B:174:LEU:HB2	1:B:194:VAL:HG22	2.01	0.41
1:G:28:MET:HA	1:G:33:MET:HG2	2.03	0.41
1:H:145:LEU:HD12	1:H:148:ILE:HD11	2.03	0.41
3:Q:54:ARG:NH1	5:Q:2082:HOH:O	2.54	0.41
3:Q:171:ILE:O	3:Q:175:SER:N	2.41	0.41
1:H:7:THR:O	1:I:65:ARG:HD2	2.20	0.41
3:Q:247:GLU:OE1	3:Q:272:ARG:NH2	2.45	0.41
1:A:244:TRP:NE1	2:E:31:ASN:HD21	2.11	0.41
1:C:5:ASN:HB3	1:C:8:PHE:CD1	2.56	0.41
2:D:88:PRO:HA	2:D:121:VAL:HB	2.02	0.41
1:H:28:MET:HA	1:H:33:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:ASN:HB3	2:E:109:LEU:HD12	2.02	0.41
3:P:215:ARG:HB3	3:P:282:ILE:HD11	2.03	0.41
2:D:48:VAL:HG13	2:D:49:VAL:HG12	2.03	0.40
3:Q:136:TRP:CE3	3:Q:136:TRP:CA	3.04	0.40
1:G:148:ILE:HD12	1:I:150:VAL:HG21	2.04	0.40
1:B:264:LYS:NZ	5:B:2083:HOH:O	2.49	0.40
1:G:26:LEU:HD21	1:H:27:TYR:CZ	2.57	0.40
2:K:34:MET:HB3	2:K:79:VAL:HG11	2.03	0.40
2:E:73:ASP:HB2	2:E:78:THR:HB	2.02	0.40
1:G:145:LEU:HD12	1:G:148:ILE:HD11	2.04	0.40
1:I:145:LEU:HD12	1:I:148:ILE:HD11	2.03	0.40
3:P:134:THR:HG21	3:P:292:LYS:HD3	2.03	0.40
3:P:181:GLU:OE1	3:P:186:ARG:NH2	2.55	0.40
3:P:136:TRP:HA	3:P:136:TRP:HE3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	264/266 (99%)	255 (97%)	9 (3%)	0	100	100
1	B	264/266 (99%)	255 (97%)	9 (3%)	0	100	100
1	C	264/266 (99%)	255 (97%)	9 (3%)	0	100	100
1	G	264/266 (99%)	254 (96%)	10 (4%)	0	100	100
1	H	264/266 (99%)	252 (96%)	12 (4%)	0	100	100
1	I	264/266 (99%)	253 (96%)	11 (4%)	0	100	100
2	D	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
2	E	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
2	F	120/123 (98%)	118 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
2	K	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
2	L	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
3	P	296/326 (91%)	285 (96%)	10 (3%)	1 (0%)	36	58
3	Q	296/326 (91%)	283 (96%)	12 (4%)	1 (0%)	36	58
4	R	373/375 (100%)	355 (95%)	18 (5%)	0	100	100
All	All	3269/3361 (97%)	3147 (96%)	120 (4%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	175	SER
3	Q	175	SER

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	228/229 (100%)	218 (96%)	10 (4%)	25	50
1	B	228/229 (100%)	221 (97%)	7 (3%)	35	63
1	C	228/229 (100%)	220 (96%)	8 (4%)	32	59
1	G	228/229 (100%)	217 (95%)	11 (5%)	23	47
1	H	228/229 (100%)	217 (95%)	11 (5%)	23	47
1	I	228/229 (100%)	217 (95%)	11 (5%)	23	47
2	D	99/100 (99%)	89 (90%)	10 (10%)	7	15
2	E	96/100 (96%)	80 (83%)	16 (17%)	2	4
2	F	98/100 (98%)	89 (91%)	9 (9%)	8	19
2	J	99/100 (99%)	84 (85%)	15 (15%)	3	5
2	K	99/100 (99%)	86 (87%)	13 (13%)	4	8
2	L	99/100 (99%)	89 (90%)	10 (10%)	7	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	264/290 (91%)	251 (95%)	13 (5%)	22	47
3	Q	264/290 (91%)	245 (93%)	19 (7%)	13	30
4	R	340/340 (100%)	317 (93%)	23 (7%)	14	32
All	All	2826/2894 (98%)	2640 (93%)	186 (7%)	15	34

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	7	THR
1	A	9	PHE
1	A	18	VAL
1	A	38	ILE
1	A	79	ASP
1	A	93	THR
1	A	124	ASP
1	A	202	ASN
1	A	233	ILE
1	B	4	LYS
1	B	7	THR
1	B	18	VAL
1	B	38	ILE
1	B	93	THR
1	B	124	ASP
1	B	233	ILE
1	C	2	THR
1	C	7	THR
1	C	18	VAL
1	C	38	ILE
1	C	80	SER
1	C	124	ASP
1	C	176	LEU
1	C	233	ILE
2	D	11	LEU
2	D	13	GLN
2	D	18	LEU
2	D	26	ARG
2	D	52	ASN
2	D	57	MET
2	D	105	SER
2	D	107	ARG

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Mol	Chain	Res	Type
2	D	108	GLU
2	D	121	VAL
2	E	3	GLN
2	E	12	VAL
2	E	19	ARG
2	E	26	ARG
2	E	27	ARG
2	E	40	LEU
2	E	47	LEU
2	E	52	ASN
2	E	57	MET
2	E	62	ASP
2	E	83	MET
2	E	86	LEU
2	E	87	LYS
2	E	90	ASP
2	E	111	ASP
2	E	121	VAL
2	F	2	VAL
2	F	37	PHE
2	F	47	LEU
2	F	48	VAL
2	F	57	MET
2	F	65	LYS
2	F	70	VAL
2	F	72	ARG
2	F	86	LEU
1	G	7	THR
1	G	9	PHE
1	G	18	VAL
1	G	38	ILE
1	G	80	SER
1	G	124	ASP
1	G	140	VAL
1	G	199	LYS
1	G	202	ASN
1	G	233	ILE
1	G	250	LYS
1	H	2	THR
1	H	7	THR
1	H	18	VAL
1	H	38	ILE

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Mol	Chain	Res	Type
1	H	74	VAL
1	H	80	SER
1	H	124	ASP
1	H	176	LEU
1	H	202	ASN
1	H	233	ILE
1	H	253	ILE
1	I	2	THR
1	I	7	THR
1	I	18	VAL
1	I	38	ILE
1	I	80	SER
1	I	124	ASP
1	I	176	LEU
1	I	183	ASN
1	I	202	ASN
1	I	233	ILE
1	I	250	LYS
2	J	2	VAL
2	J	5	GLN
2	J	11	LEU
2	J	12	VAL
2	J	13	GLN
2	J	19	ARG
2	J	26	ARG
2	J	38	ARG
2	J	40	LEU
2	J	52	ASN
2	J	57	MET
2	J	79	VAL
2	J	81	LEU
2	J	89	GLU
2	J	93	ILE
2	K	11	LEU
2	K	12	VAL
2	K	19	ARG
2	K	26	ARG
2	K	47	LEU
2	K	52	ASN
2	K	57	MET
2	K	70	VAL
2	K	83	MET

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Mol	Chain	Res	Type
2	K	86	LEU
2	K	93	ILE
2	K	107	ARG
2	K	121	VAL
2	L	2	VAL
2	L	11	LEU
2	L	20	LEU
2	L	39	GLN
2	L	40	LEU
2	L	47	LEU
2	L	52	ASN
2	L	57	MET
2	L	86	LEU
2	L	93	ILE
3	P	11	LEU
3	P	45	SER
3	P	53	THR
3	P	54	ARG
3	P	56	ILE
3	P	92	VAL
3	P	176	TYR
3	P	186	ARG
3	P	193	LYS
3	P	202	ILE
3	P	258	LEU
3	P	263	VAL
3	P	298	VAL
3	Q	11	LEU
3	Q	53	THR
3	Q	54	ARG
3	Q	56	ILE
3	Q	66	GLU
3	Q	92	VAL
3	Q	127	LYS
3	Q	136	TRP
3	Q	176	TYR
3	Q	193	LYS
3	Q	194	GLU
3	Q	196	ILE
3	Q	228	VAL
3	Q	242	THR
3	Q	248	THR

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Mol	Chain	Res	Type
3	Q	258	LEU
3	Q	263	VAL
3	Q	270	ARG
3	Q	298	VAL
4	R	2	LEU
4	R	21	SER
4	R	26	LYS
4	R	40	GLN
4	R	41	VAL
4	R	52	LEU
4	R	77	VAL
4	R	79	ILE
4	R	83	LEU
4	R	85	LYS
4	R	89	LEU
4	R	102	GLU
4	R	121	VAL
4	R	137	LEU
4	R	160	LYS
4	R	175	VAL
4	R	190	THR
4	R	219	THR
4	R	229	THR
4	R	231	ASP
4	R	306	LEU
4	R	310	LYS
4	R	337	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	71	ASN
1	A	82	ASN
1	A	106	ASN
1	A	172	ASN
1	A	196	ASN
1	B	71	ASN
1	B	196	ASN
1	C	5	ASN
1	C	48	ASN
1	C	54	GLN

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Mol	Chain	Res	Type
1	C	71	ASN
1	C	172	ASN
1	C	196	ASN
1	C	198	GLN
2	D	31	ASN
2	D	39	GLN
2	D	118	GLN
2	E	31	ASN
2	E	52	ASN
2	E	77	ASN
2	E	84	ASN
2	F	31	ASN
1	G	48	ASN
1	G	52	ASN
1	G	71	ASN
1	G	82	ASN
1	G	95	ASN
1	G	172	ASN
1	G	196	ASN
1	H	48	ASN
1	H	54	GLN
1	H	71	ASN
1	H	172	ASN
1	H	175	GLN
1	H	196	ASN
1	H	198	GLN
1	I	48	ASN
1	I	71	ASN
1	I	172	ASN
2	J	5	GLN
2	J	13	GLN
2	J	39	GLN
2	J	77	ASN
2	J	82	GLN
2	J	84	ASN
2	J	118	GLN
2	K	52	ASN
2	K	118	GLN
2	L	31	ASN
2	L	52	ASN
2	L	118	GLN
3	P	46	ASN

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Mol	Chain	Res	Type
3	P	148	GLN
3	P	235	GLN
3	P	278	GLN
3	Q	23	ASN
3	Q	241	ASN
3	Q	278	GLN
4	R	40	GLN
4	R	43	ASN
4	R	143	ASN
4	R	173	HIS
4	R	184	GLN
4	R	186	GLN
4	R	207	ASN
4	R	267	ASN
4	R	302	ASN

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	266/266 (100%)	0.40	11 (4%) 41 36	53, 82, 115, 135	0
1	B	266/266 (100%)	-0.08	1 (0%) 88 86	41, 63, 86, 118	0
1	C	266/266 (100%)	-0.00	7 (2%) 57 51	36, 57, 110, 146	0
1	G	266/266 (100%)	-0.42	2 (0%) 82 80	28, 42, 79, 111	0
1	H	266/266 (100%)	-0.41	4 (1%) 72 68	27, 43, 90, 113	0
1	I	266/266 (100%)	-0.53	1 (0%) 88 86	25, 40, 83, 103	0
2	D	122/123 (99%)	0.40	3 (2%) 58 52	61, 80, 97, 108	0
2	E	122/123 (99%)	1.54	35 (28%) 1 1	102, 138, 158, 170	0
2	F	122/123 (99%)	1.67	40 (32%) 1 1	112, 156, 177, 197	0
2	J	122/123 (99%)	1.43	24 (19%) 3 2	72, 131, 152, 168	1 (0%)
2	K	122/123 (99%)	1.17	14 (11%) 9 7	80, 119, 142, 159	0
2	L	122/123 (99%)	0.83	9 (7%) 20 16	72, 101, 129, 145	0
3	P	298/326 (91%)	-0.88	2 (0%) 84 82	20, 34, 57, 89	0
3	Q	298/326 (91%)	-0.75	5 (1%) 69 64	23, 40, 63, 93	0
4	R	375/375 (100%)	-1.13	0 100 100	17, 26, 45, 77	0
All	All	3299/3361 (98%)	-0.10	158 (4%) 35 30	17, 57, 143, 197	1 (0%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	2	VAL	5.7
2	E	35	GLY	5.2
2	F	97	ALA	5.0
2	F	109	LEU	4.9
2	K	2	VAL	4.8
2	L	40	LEU	4.7
1	H	267	TRP	4.7

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Mol	Chain	Res	Type	RSRZ
2	E	47	LEU	4.6
2	J	35	GLY	4.5
1	A	267	TRP	4.3
1	I	267	TRP	4.2
2	E	18	LEU	4.2
2	J	50	ALA	4.0
2	K	112	GLY	4.0
1	A	254	ALA	3.9
2	F	2	VAL	3.9
1	C	267	TRP	3.8
1	B	267	TRP	3.8
2	F	34	MET	3.7
3	Q	118	TYR	3.6
2	J	18	LEU	3.6
1	G	267	TRP	3.5
2	J	40	LEU	3.5
2	E	41	ALA	3.5
2	J	51	LEU	3.4
2	E	40	LEU	3.4
2	D	2	VAL	3.4
2	J	43	LYS	3.3
2	F	53	PHE	3.3
2	E	50	ALA	3.3
2	L	41	ALA	3.3
2	E	20	LEU	3.2
1	A	199	LYS	3.2
2	F	81	LEU	3.2
2	E	94	TYR	3.2
2	F	103	PHE	3.1
2	E	110	TYR	3.1
2	F	40	LEU	3.1
2	F	11	LEU	3.0
2	K	97	ALA	3.0
2	F	77	ASN	3.0
2	J	57	MET	3.0
1	C	266	ALA	3.0
2	E	14	ALA	3.0
2	E	12	VAL	3.0
2	F	20	LEU	2.9
2	E	97	ALA	2.9
2	F	18	LEU	2.9
2	J	11	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	93	ILE	2.9
2	E	104	SER	2.8
3	Q	1	GLY	2.8
2	F	80	TYR	2.8
2	F	117	THR	2.8
2	F	70	VAL	2.8
2	E	71	SER	2.8
2	F	12	VAL	2.8
2	F	33	CYS	2.7
2	F	35	GLY	2.7
2	F	57	MET	2.7
2	F	111	ASP	2.7
2	F	110	TYR	2.7
1	A	198	GLN	2.7
2	F	119	VAL	2.7
3	P	118	TYR	2.7
2	J	16	GLY	2.7
1	C	242	THR	2.7
2	E	49	VAL	2.7
2	J	37	PHE	2.7
2	J	20	LEU	2.7
2	L	43	LYS	2.6
3	Q	120	LYS	2.6
1	A	201	TRP	2.6
2	J	97	ALA	2.6
1	H	199	LYS	2.6
2	F	61	ALA	2.6
2	J	86	LEU	2.6
2	F	65	LYS	2.6
3	Q	209	LYS	2.6
2	L	45	PRO	2.6
2	E	105	SER	2.6
2	K	111	ASP	2.6
2	E	57	MET	2.6
2	E	19	ARG	2.6
2	J	88	PRO	2.6
2	F	51	LEU	2.5
2	F	37	PHE	2.5
2	E	45	PRO	2.5
1	H	254	ALA	2.5
2	E	37	PHE	2.5
2	E	98	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	105	SER	2.4
2	F	113	TRP	2.4
2	J	10	GLY	2.4
2	F	43	LYS	2.4
2	F	32	TRP	2.4
2	K	70	VAL	2.4
2	K	41	ALA	2.4
2	F	31	ASN	2.3
2	L	74	SER	2.3
2	F	93	ILE	2.3
2	J	120	THR	2.3
2	L	77	ASN	2.3
1	A	252	PRO	2.3
2	J	45	PRO	2.3
2	E	16	GLY	2.3
2	J	47	LEU	2.3
2	J	94	TYR	2.3
2	K	85	SER	2.3
2	E	79	VAL	2.3
1	C	199	LYS	2.3
2	K	45	PRO	2.3
2	L	21	SER	2.3
2	E	109	LEU	2.3
2	F	21	SER	2.2
2	F	118	GLN	2.2
1	A	246	ALA	2.2
2	E	83	MET	2.2
2	E	112	GLY	2.2
3	Q	117	GLY	2.2
2	K	40	LEU	2.2
1	C	200	GLY	2.2
2	F	54	ASP	2.2
2	J	102	GLY	2.2
1	A	190	PHE	2.2
1	C	201	TRP	2.2
2	L	76	LYS	2.2
2	F	49	VAL	2.2
2	E	103	PHE	2.2
1	A	225	ALA	2.1
2	F	14	ALA	2.1
2	E	39	GLN	2.1
2	K	43	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	203	MET	2.1
2	J	79	VAL	2.1
3	P	120	LYS	2.1
2	F	112	GLY	2.1
2	E	2	VAL	2.1
1	C	244	TRP	2.1
2	E	113	TRP	2.1
2	K	109	LEU	2.1
2	E	95	TYR	2.1
2	J	53	PHE	2.1
1	A	256	ARG	2.1
2	E	65	LYS	2.1
2	D	57	MET	2.1
2	E	34	MET	2.1
2	K	20	LEU	2.1
2	J	49	VAL	2.1
2	F	30	SER	2.0
1	G	199	LYS	2.0
2	K	113	TRP	2.0
2	E	10	GLY	2.0
2	D	49	VAL	2.0
2	F	79	VAL	2.0
1	A	244	TRP	2.0
2	E	51	LEU	2.0
2	K	110	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.