Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:26 AM GMT

PDB ID	:	2WZP
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

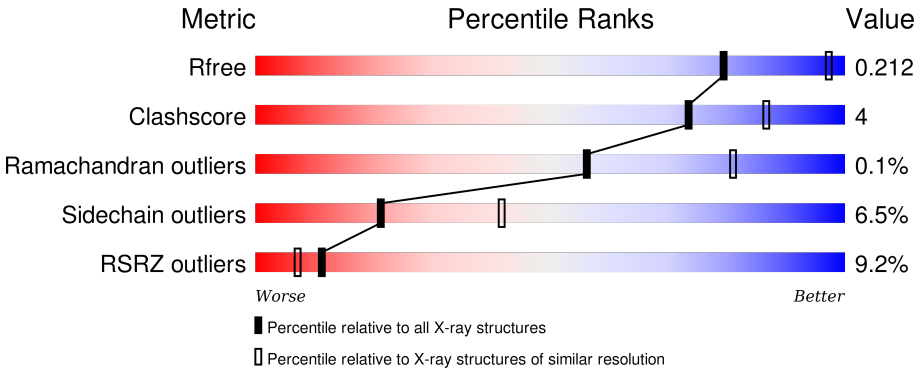
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	7% 91% 9%
1	B	266	5% 91% 8%
1	C	266	3% 91% 9%
1	G	266	2% 87% 13%
1	H	266	2% 89% 11%

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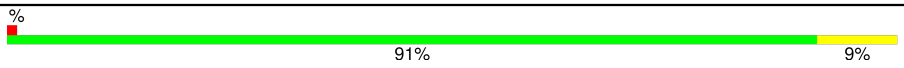
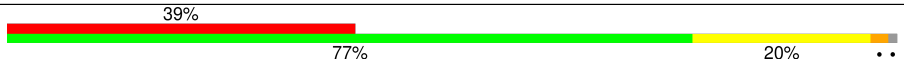
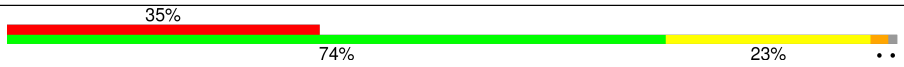
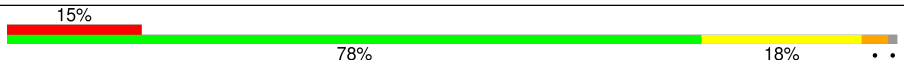
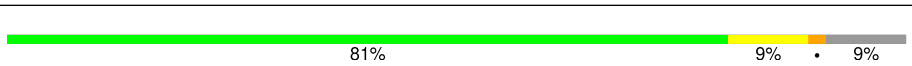
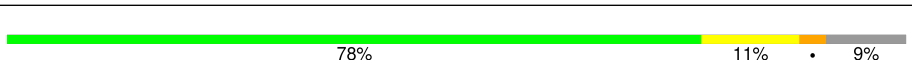
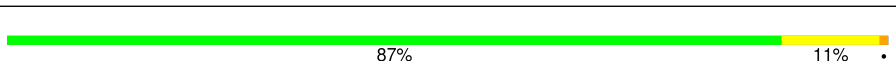
Mol	Chain	Length	Quality of chain
1	I	266	
2	D	123	
2	E	123	
2	F	123	
2	J	123	
2	K	123	
2	L	123	
3	P	326	
3	Q	326	
4	R	375	

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.

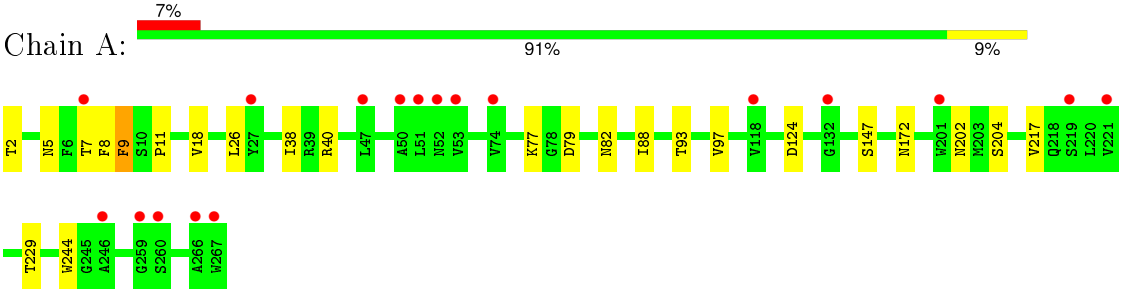
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	B	85	Total	O	0	0
			85	85		
5	C	112	Total	O	0	0
			112	112		
5	D	11	Total	O	0	0
			11	11		
5	E	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		
5	G	199	Total	O	0	0
			199	199		
5	H	156	Total	O	0	0
			156	156		
5	I	192	Total	O	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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

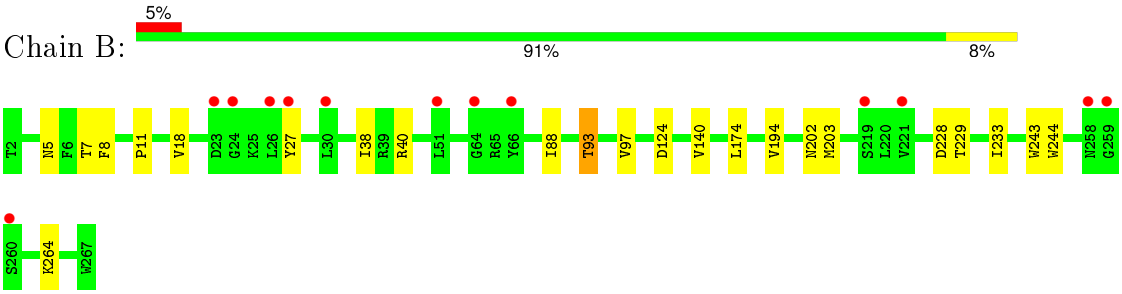
- Molecule 1: PUTATIVE RECEPTOR BINDING PROTEIN

Chain A:



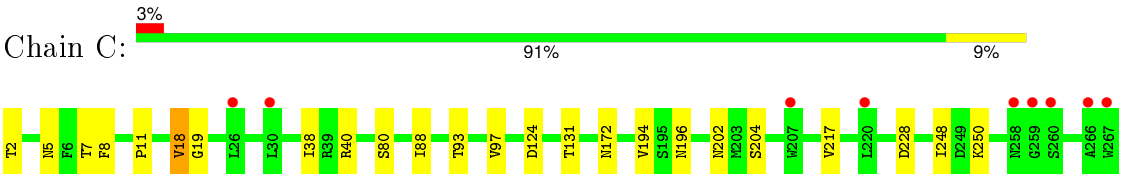
- Molecule 1: PUTATIVE RECEPTOR BINDING PROTEIN

Chain B:



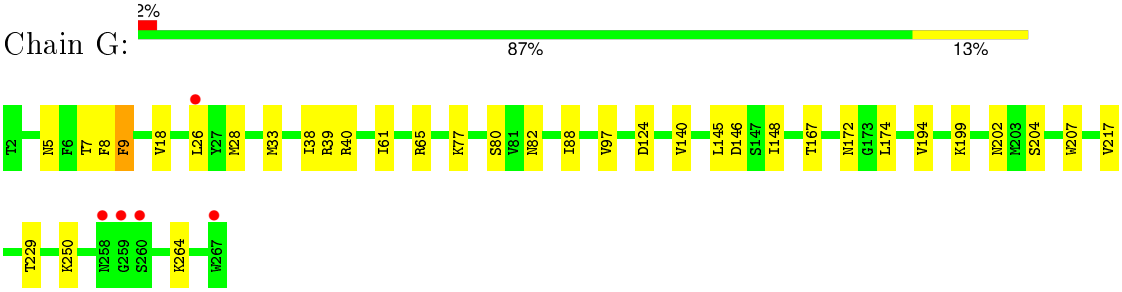
- Molecule 1: PUTATIVE RECEPTOR BINDING PROTEIN

Chain C:



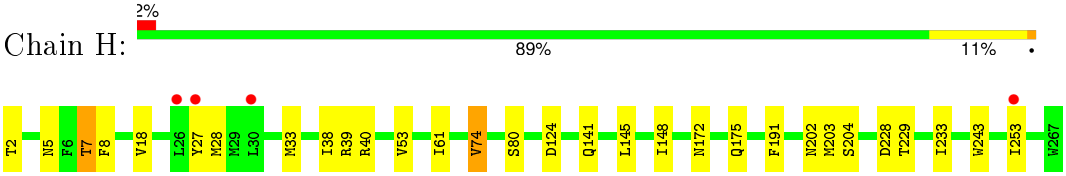
- Molecule 1: PUTATIVE RECEPTOR BINDING PROTEIN

Chain G:



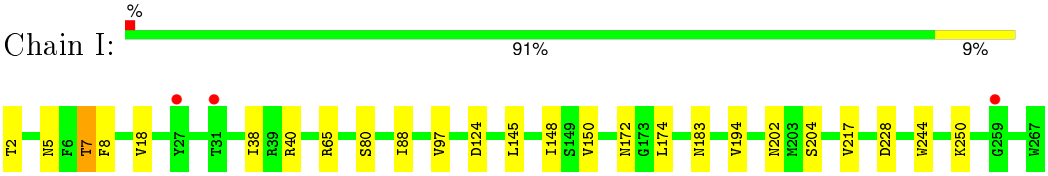
• Molecule 1: PUTATIVE RECEPTOR BINDING PROTEIN

Chain H:



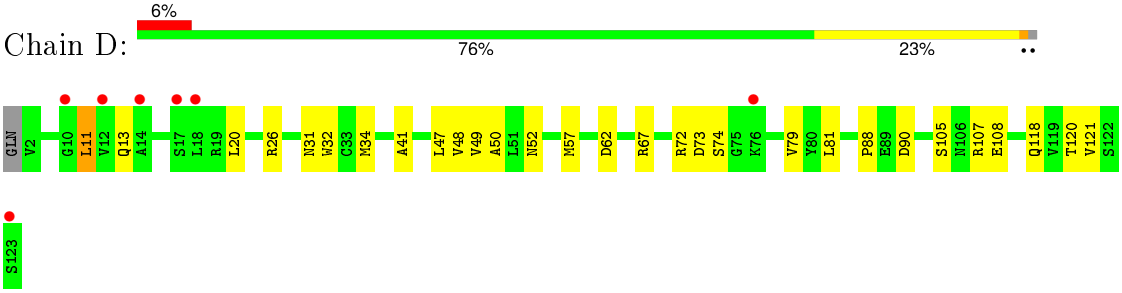
• Molecule 1: PUTATIVE RECEPTOR BINDING PROTEIN

Chain I:



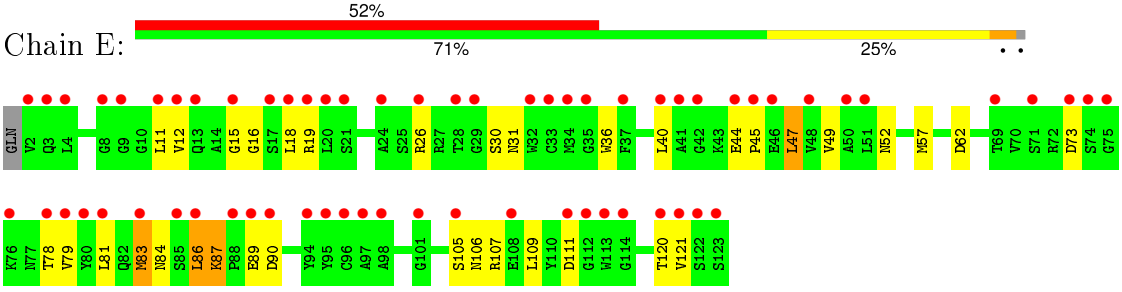
• Molecule 2: CAMELID VHH5

Chain D:



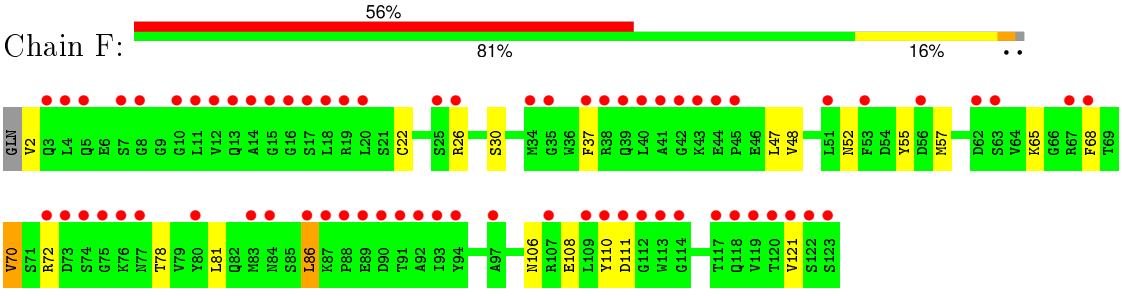
• Molecule 2: CAMELID VHH5

Chain E:



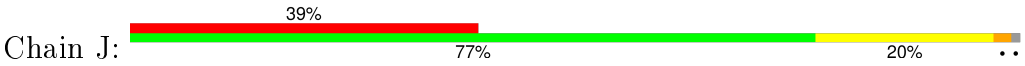
• Molecule 2: CAMELID VHH5

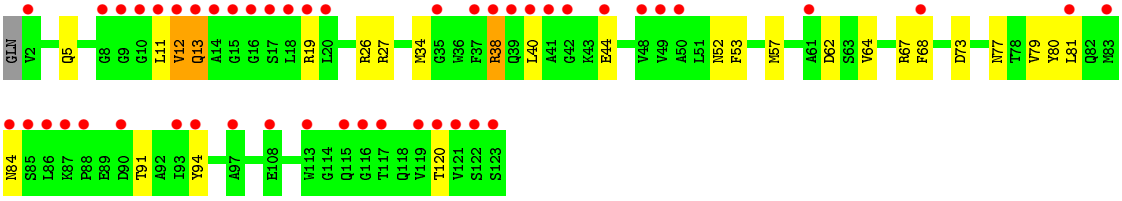
Chain F:



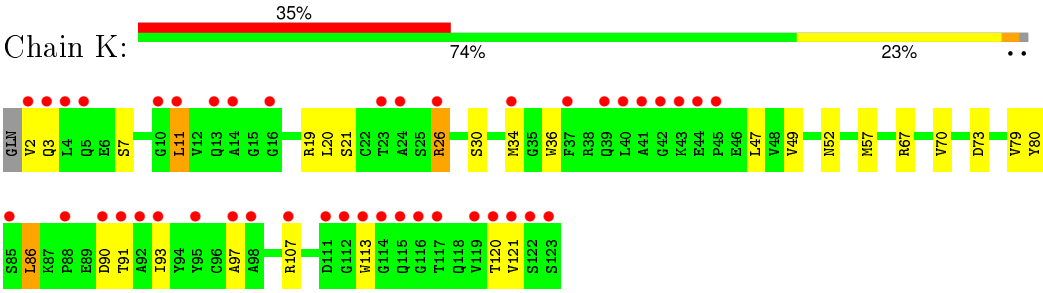
• Molecule 2: CAMELID VHH5

Chain J:

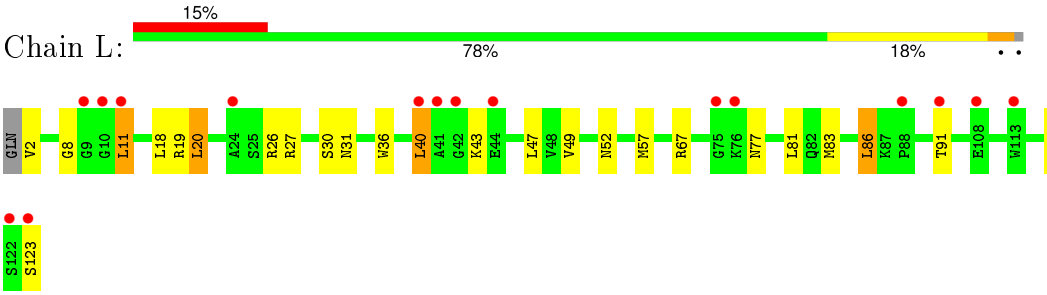




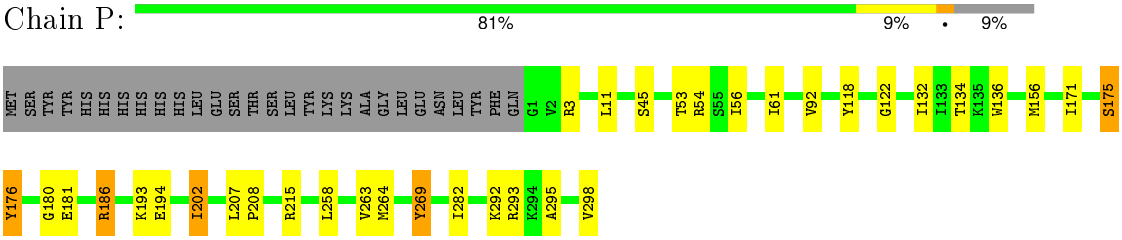
• Molecule 2: CAMELID VHH5



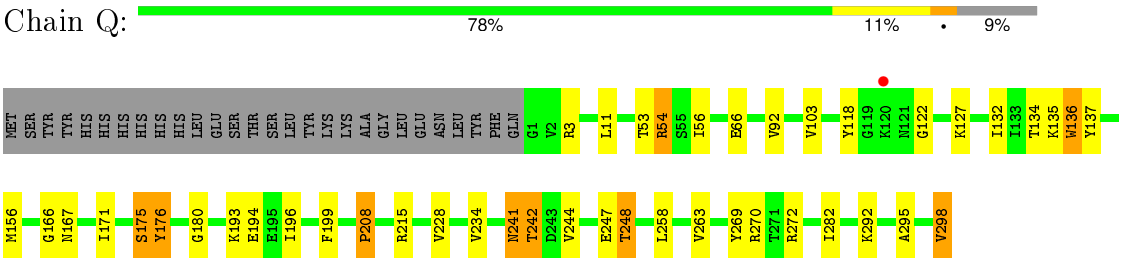
• Molecule 2: CAMELID VHH5



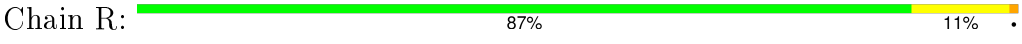
• Molecule 3: LACTOCOCCAL PHAGE P2 ORF15

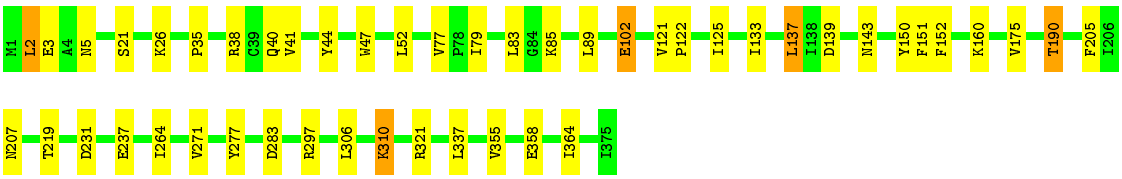


• Molecule 3: LACTOCOCCAL PHAGE P2 ORF15



• Molecule 4: LACTOCOCCAL PHAGE P2 ORF16




M1
L2
E3
A4
N5
S21
K26
P35
R38
C39
Q40
V41
Y44
W47
L52
V77
P78
I79
L83
Q84
K85
L89
E102
V121
P122
I125
I133
L137
I138
D139
N143
Y150
F151
F152
K160
V175
T190
F205
I206
N207
T219
D231
E237
I264
V271
Y277
D283
R297
L306
K310
R321
L337
V355
E358
I364
I375

4 Data and refinement statistics (i)

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 37.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.07-2.60) 99.3 (37.91-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.179 , 0.208 0.184 , 0.212	Depositor DCC
R_{free} test set	3689 reflections (2.05%)	DCC
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 183300 reflections	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.38	0/2064	0.64	0/2813
1	B	0.38	0/2064	0.64	0/2813
1	C	0.39	0/2064	0.63	0/2813
1	G	0.42	0/2064	0.67	0/2813
1	H	0.41	0/2064	0.67	0/2813
1	I	0.42	0/2064	0.66	0/2813
2	D	0.39	0/956	0.63	0/1289
2	E	0.43	0/940	0.73	0/1271
2	F	0.43	0/948	0.67	0/1278
2	J	0.43	0/956	0.67	0/1289
2	K	0.41	0/956	0.66	0/1289
2	L	0.42	0/956	0.66	0/1289
3	P	0.52	0/2485	0.79	0/3356
3	Q	0.50	0/2485	0.79	1/3356 (0.0%)
4	R	0.57	0/3094	0.81	0/4208
All	All	0.45	0/26160	0.71	1/35503 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	208	PRO	N-CA-C	5.52	126.44	112.10

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	17	0
1	B	2024	0	1983	18	0
1	C	2024	0	1983	16	0
1	G	2024	0	1983	19	0
1	H	2024	0	1983	16	0
1	I	2024	0	1983	11	0
2	D	938	0	891	12	0
2	E	922	0	858	17	0
2	F	931	0	884	8	0
2	J	938	0	891	10	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	209	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 (209) 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:B:203:MET:HE1	1:B:243:TRP:HE3	1.40	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:MET:HE1	1:H:243:TRP:HE3	1.48	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
3:P:156:MET:O	3:P:176:TYR:HA	1.86	0.75
3:Q:156:MET:O	3:Q:176:TYR:HA	1.86	0.74
3:P:175:SER:OG	3:P:176:TYR:N	2.21	0.73
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: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:175:SER:OG	3:Q:176:TYR:N	2.23	0.70
3:Q:171:ILE:H	3:Q:175:SER:HA	1.57	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
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
3:Q:136:TRP:HB2	3:Q:295:ALA:O	1.97	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
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
4:R:102:GLU:CD	4:R:102:GLU:H	1.99	0.62
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
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
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: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
4:R:237:GLU:CD	4:R:321:ARG:HH22	2.05	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:B:203:MET:HE3	1:B:233:ILE:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:D:32:TRP:HE1	2:D:34:MET:HE3	1.73	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
3:Q:132:ILE:HG23	3:Q:135:LYS:HB2	1.92	0.52
1:G:88:ILE:HG12	1:G:97:VAL:HG22	1.91	0.52
1:A:217:VAL:HB	2:E:30:SER:CB	2.40	0.52
4:R:47:TRP:CZ3	4:R:364:ILE:HD11	2.45	0.51
1:A:77:LYS:H	1:A:82:ASN:ND2	2.06	0.51
2:L:67:ARG:HH21	2:L:86:LEU:HA	1.75	0.51
2:L:8:GLY:O	2:L:117:THR:HG21	2.09	0.51
1:G:229:THR:HB	1:H:228:ASP:HB2	1.93	0.51
2:L:20:LEU:HD12	2:L:81:LEU:HB3	1.92	0.51
2:K:20:LEU:HD12	2:K:81:LEU:HD23	1.91	0.51
1:C:18:VAL:O	3:Q:167:ASN:HA	2.11	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
1:A:9:PHE:HB2	3:Q:180:GLY:HA2	1.94	0.50
3:Q:171:ILE:H	3:Q:175:SER:CA	2.23	0.50
1:H:172:ASN:HD21	1:H:204:SER:H	1.57	0.50
4:R:190:THR:HB	4:R:207:ASN:HD21	1.77	0.49
3:P:118:TYR:HB3	3:P:122:GLY:HA2	1.94	0.49
2:F:68:PHE:HB3	2:F:81:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:91:THR:HG23	2:L:120:THR:HA	1.95	0.49
1:C:172:ASN:ND2	1:C:204:SER:H	2.11	0.49
1:A:229:THR:HB	1:B:228:ASP:HB2	1.93	0.49
3:Q:3:ARG:HD2	3:Q:3:ARG:C	2.33	0.48
2:K:67:ARG:NH2	2:K:90:ASP:OD2	2.46	0.48
3:Q:134:THR:HG22	3:Q:137:TYR:CD2	2.48	0.48
1:B:203:MET:CE	1:B:233:ILE:CG2	2.89	0.48
3:Q:241:ASN:HD22	3:Q:242:THR:N	2.11	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
2:K:73:ASP:HB2	2:K:80:TYR:HE2	1.78	0.48
2:F:22:CYS:O	2:F:78:THR:HA	2.13	0.48
1:I:5:ASN:HB3	1:I:8:PHE:CD1	2.48	0.48
2:E:49:VAL:HG21	2:E:81:LEU:HD13	1.95	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:A:88:ILE:HG12	1:A:97:VAL:HG22	1.95	0.48
1:G:146:ASP:HB3	1:H:141:GLN:O	2.13	0.48
2:E:44:GLU:HB3	2:E:45:PRO:HD2	1.96	0.48
3:Q:136:TRP:CE3	3:Q:136:TRP:HA	2.48	0.47
2:F:86:LEU:HD22	2:F:121:VAL:HG21	1.95	0.47
1:H:5:ASN:HB3	1:H:8:PHE:CD1	2.50	0.47
1:B:203:MET:HE3	1:B:233:ILE:HG21	1.96	0.47
2:K:2:VAL:HG11	2:K:26:ARG:CG	2.44	0.47
1:B:203:MET:HE1	1:B:233:ILE:HG22	1.97	0.47
1:H:203:MET:CE	1:H:233:ILE:HG22	2.45	0.47
2:D:41:ALA:HA	1:G:207:TRP:CD1	2.50	0.46
1:B:11:PRO:HG3	1:C:93:THR:HB	1.97	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
2:K:11:LEU:HG	2:K:120:THR:HB	1.98	0.46
1:G:9:PHE:HB2	3:P:180:GLY:HA2	1.97	0.46
4:R:139:ASP:H	4:R:143:ASN:ND2	2.13	0.46
3:Q:215:ARG:HB3	3:Q:282:ILE:HD11	1.97	0.46
3:P:171:ILE:H	3:P:175:SER:CA	2.27	0.46
2:F:70:VAL:HG13	2:F:81:LEU:HD13	1.98	0.46
1:A:11:PRO:HG2	1:B:93:THR:CG2	2.45	0.46
4:R:47:TRP:CE3	4:R:355:VAL:HB	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:LEU:HB2	1:I:194:VAL:HG22	1.98	0.46
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
4:R:190:THR:HB	4:R:207:ASN:ND2	2.31	0.45
1:B:229:THR:HB	1:C:228:ASP:HB2	1.99	0.45
2:K:97:ALA:HB2	2:K:113:TRP:CZ3	2.51	0.45
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.49	0.45
4:R:150:TYR:HD1	4:R:152:PHE:HE1	1.64	0.45
1:I:217:VAL:HB	2:L:30:SER:CB	2.47	0.45
4:R:297:ARG:NH1	5:R:2475:HOH:O	2.50	0.45
4:R:3:GLU:OE2	4:R:38:ARG:HD2	2.17	0.45
2:D:72:ARG:NH2	2:D:74:SER:O	2.50	0.45
1:A:26:LEU:HD21	1:B:27:TYR:CZ	2.52	0.45
3:P:3:ARG:HD2	3:P:3:ARG:C	2.38	0.44
2:J:67:ARG:HG2	2:J:84:ASN:O	2.18	0.44
3:Q:134:THR:HG21	3:Q:292:LYS:HE2	2.00	0.44
1:A:147:SER:HB2	1:B:140:VAL:HG21	2.00	0.44
1:G:217:VAL:HB	2:K:30:SER:CB	2.48	0.44
1:G:174:LEU:HB2	1:G:194:VAL:HG22	1.99	0.44
1:C:217:VAL:HB	2:F:30:SER:CB	2.48	0.44
4:R:277:TYR:OH	4:R:283:ASP:OD1	2.30	0.44
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
4:R:297:ARG:NH2	5:R:2477:HOH:O	2.41	0.43
1:B:88:ILE:HG12	1:B:97:VAL:HG22	2.00	0.43
4:R:47:TRP:CZ3	4:R:355:VAL:HB	2.53	0.43
2:J:91:THR:HG23	2:J:120:THR:HA	2.00	0.43
1:G:65:ARG:HD2	1:I:7:THR:O	2.19	0.43
2:E:47:LEU:HD12	2:E:105:SER:HA	2.01	0.43
1:C:172:ASN:HD21	1:C:204:SER:H	1.65	0.43
2:L:27:ARG:HG3	2:L:77:ASN:HD21	1.84	0.43
2:L:11:LEU:HA	2:L:120:THR:O	2.18	0.43
2:E:16:GLY:HA2	2:E:84:ASN:HD22	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:5:ASN:HB3	4:R:35:PRO:HG3	2.01	0.42
2:L:36:TRP:CZ3	2:L:81:LEU:HB2	2.54	0.42
2:K:49:VAL:HG11	2:K:81:LEU:HD13	2.01	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:34:MET:HB3	2:D:79:VAL:HG11	2.02	0.42
2:D:11:LEU:HG	2:D:120:THR:HB	2.01	0.42
1:H:203:MET:HE1	1:H:233:ILE:HG22	2.02	0.42
3:P:207:LEU:HA	3:P:208:PRO:HD3	1.95	0.42
1:H:39:ARG:HB2	1:H:61:ILE:HB	2.01	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
2:E:18:LEU:HB2	2:E:83:MET:HE1	2.02	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
3:Q:171:ILE:O	3:Q:175:SER:N	2.41	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
1:G:28:MET:HA	1:G:33:MET:HG2	2.03	0.41
3:Q:247:GLU:OE1	3:Q:272:ARG:NH2	2.45	0.41
1:H:7:THR:O	1:I:65:ARG:HD2	2.20	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
1:H:203:MET:CE	1:H:233:ILE:CG2	2.98	0.41
3:P:215:ARG:HB3	3:P:282:ILE:HD11	2.03	0.41
2:E:106:ASN:HB3	2:E:109:LEU:HD12	2.02	0.41
3:Q:136:TRP:CE3	3:Q:136:TRP:CA	3.04	0.40
2:D:48:VAL:HG13	2:D:49:VAL:HG12	2.03	0.40
1:G:148:ILE:HD12	1:I:150:VAL:HG21	2.04	0.40
1:G:26:LEU:HD21	1:H:27:TYR:CZ	2.57	0.40
1:B:264:LYS:NZ	5:B:2083:HOH:O	2.49	0.40
2:K:34:MET:HB3	2:K:79:VAL:HG11	2.03	0.40
1:G:145:LEU:HD12	1:G:148:ILE:HD11	2.04	0.40
2:E:73:ASP:HB2	2:E:78:THR:HB	2.02	0.40
3:P:181:GLU:OE1	3:P:186:ARG:NH2	2.55	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:136:TRP:HA	3:P:136:TRP:HE3	1.86	0.40
2:L:18:LEU:HB3	2:L:83:MET:HE3	2.03	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	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
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%)	46	72
3	Q	296/326 (91%)	283 (96%)	12 (4%)	1 (0%)	46	72
4	R	373/375 (100%)	355 (95%)	18 (5%)	0	100	100
All	All	3269/3361 (97%)	3147 (96%)	120 (4%)	2 (0%)	56	81

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%)	219 (96%)	9 (4%)	39	68
1	B	228/229 (100%)	221 (97%)	7 (3%)	47	76
1	C	228/229 (100%)	220 (96%)	8 (4%)	43	71
1	G	228/229 (100%)	217 (95%)	11 (5%)	31	58
1	H	228/229 (100%)	218 (96%)	10 (4%)	35	63
1	I	228/229 (100%)	218 (96%)	10 (4%)	35	63
2	D	99/100 (99%)	89 (90%)	10 (10%)	9	17
2	E	96/100 (96%)	83 (86%)	13 (14%)	5	8
2	F	98/100 (98%)	86 (88%)	12 (12%)	6	11
2	J	99/100 (99%)	85 (86%)	14 (14%)	4	7
2	K	99/100 (99%)	88 (89%)	11 (11%)	8	13
2	L	99/100 (99%)	88 (89%)	11 (11%)	8	13
3	P	264/290 (91%)	250 (95%)	14 (5%)	28	53
3	Q	264/290 (91%)	243 (92%)	21 (8%)	15	29
4	R	340/340 (100%)	318 (94%)	22 (6%)	21	42
All	All	2826/2894 (98%)	2643 (94%)	183 (6%)	21	42

All (183) 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	40	ARG
1	A	79	ASP
1	A	124	ASP
1	A	202	ASN
1	B	7	THR
1	B	18	VAL
1	B	38	ILE
1	B	40	ARG
1	B	93	THR

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Mol	Chain	Res	Type
1	B	124	ASP
1	B	202	ASN
1	C	2	THR
1	C	7	THR
1	C	18	VAL
1	C	38	ILE
1	C	40	ARG
1	C	80	SER
1	C	124	ASP
1	C	202	ASN
2	D	11	LEU
2	D	13	GLN
2	D	26	ARG
2	D	52	ASN
2	D	57	MET
2	D	62	ASP
2	D	73	ASP
2	D	105	SER
2	D	107	ARG
2	D	108	GLU
2	E	12	VAL
2	E	19	ARG
2	E	26	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	107	ARG
2	E	111	ASP
2	F	2	VAL
2	F	26	ARG
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

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Mol	Chain	Res	Type
2	F	86	LEU
2	F	110	TYR
2	F	111	ASP
1	G	7	THR
1	G	9	PHE
1	G	18	VAL
1	G	38	ILE
1	G	40	ARG
1	G	80	SER
1	G	124	ASP
1	G	140	VAL
1	G	199	LYS
1	G	202	ASN
1	G	250	LYS
1	H	2	THR
1	H	7	THR
1	H	18	VAL
1	H	38	ILE
1	H	40	ARG
1	H	74	VAL
1	H	80	SER
1	H	124	ASP
1	H	202	ASN
1	H	253	ILE
1	I	2	THR
1	I	7	THR
1	I	18	VAL
1	I	38	ILE
1	I	40	ARG
1	I	80	SER
1	I	124	ASP
1	I	183	ASN
1	I	202	ASN
1	I	250	LYS
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

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Mol	Chain	Res	Type
2	J	44	GLU
2	J	52	ASN
2	J	57	MET
2	J	62	ASP
2	J	79	VAL
2	J	81	LEU
2	K	11	LEU
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	86	LEU
2	K	93	ILE
2	K	107	ARG
2	K	121	VAL
2	L	2	VAL
2	L	11	LEU
2	L	19	ARG
2	L	20	LEU
2	L	26	ARG
2	L	40	LEU
2	L	47	LEU
2	L	52	ASN
2	L	57	MET
2	L	86	LEU
2	L	123	SER
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	269	TYR
3	P	298	VAL

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Mol	Chain	Res	Type
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	241	ASN
3	Q	242	THR
3	Q	248	THR
3	Q	258	LEU
3	Q	263	VAL
3	Q	269	TYR
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	231	ASP
4	R	306	LEU
4	R	310	LYS

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Mol	Chain	Res	Type
4	R	337	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	82	ASN
1	A	172	ASN
1	A	175	GLN
1	A	196	ASN
1	B	5	ASN
1	B	71	ASN
1	B	175	GLN
1	B	196	ASN
1	C	5	ASN
1	C	71	ASN
1	C	172	ASN
1	C	175	GLN
1	C	196	ASN
2	D	31	ASN
2	D	52	ASN
2	D	118	GLN
2	E	31	ASN
2	E	52	ASN
2	E	84	ASN
2	F	31	ASN
2	F	52	ASN
1	G	71	ASN
1	G	82	ASN
1	G	172	ASN
1	G	196	ASN
1	H	48	ASN
1	H	71	ASN
1	H	172	ASN
1	H	175	GLN
1	H	196	ASN
1	I	71	ASN
1	I	172	ASN
2	J	5	GLN
2	J	13	GLN
2	J	77	ASN
2	K	52	ASN

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Mol	Chain	Res	Type
2	L	31	ASN
2	L	52	ASN
3	P	278	GLN
3	Q	241	ASN
3	Q	278	GLN
4	R	43	ASN
4	R	143	ASN
4	R	267	ASN

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 carbohydrates 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, 95^{th} 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%)	0.30	18 (6%) 20 15	53, 82, 115, 135	0
1	B	266/266 (100%)	-0.02	13 (4%) 33 26	41, 63, 86, 118	0
1	C	266/266 (100%)	-0.09	9 (3%) 49 41	36, 57, 110, 146	0
1	G	266/266 (100%)	-0.30	5 (1%) 70 64	28, 42, 79, 111	0
1	H	266/266 (100%)	-0.15	4 (1%) 76 71	27, 43, 90, 113	0
1	I	266/266 (100%)	-0.37	3 (1%) 82 79	25, 40, 83, 103	0
2	D	122/123 (99%)	0.24	7 (5%) 27 20	61, 80, 97, 108	0
2	E	122/123 (99%)	2.25	64 (52%) 0 0	102, 138, 158, 170	0
2	F	122/123 (99%)	2.72	69 (56%) 0 0	112, 156, 177, 197	0
2	J	122/123 (99%)	1.77	48 (39%) 0 0	93, 131, 152, 168	1 (0%)
2	K	122/123 (99%)	1.60	43 (35%) 0 0	80, 119, 142, 159	0
2	L	122/123 (99%)	0.60	18 (14%) 3 2	72, 101, 129, 145	0
3	P	298/326 (91%)	-0.65	0 100 100	20, 34, 57, 89	0
3	Q	298/326 (91%)	-0.70	1 (0%) 94 93	23, 40, 63, 93	0
4	R	375/375 (100%)	-0.57	0 100 100	17, 26, 45, 77	0
All	All	3299/3361 (98%)	0.10	302 (9%) 11 7	17, 57, 143, 197	1 (0%)

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	109	LEU	9.7
2	F	11	LEU	9.4
2	E	18	LEU	8.6
2	K	112	GLY	8.6
2	K	114	GLY	8.1
2	E	35	GLY	8.1
2	F	121	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
2	E	19	ARG	6.6
2	F	123	SER	6.4
2	L	41	ALA	6.3
2	F	76	LYS	6.3
2	K	40	LEU	6.1
2	K	123	SER	6.1
2	E	17	SER	5.9
2	J	11	LEU	5.9
2	J	37	PHE	5.7
2	F	14	ALA	5.7
2	F	16	GLY	5.6
2	F	111	ASP	5.6
2	F	119	VAL	5.6
2	J	120	THR	5.5
2	J	12	VAL	5.5
2	F	18	LEU	5.4
2	F	13	GLN	5.4
2	K	41	ALA	5.4
2	F	15	GLY	5.3
2	F	41	ALA	5.3
2	J	9	GLY	5.3
2	J	41	ALA	5.1
2	F	112	GLY	5.1
2	F	34	MET	5.1
2	E	98	ALA	5.0
2	E	13	GLN	5.0
2	E	50	ALA	4.9
2	E	24	ALA	4.9
2	E	123	SER	4.9
2	F	88	PRO	4.9
2	E	45	PRO	4.9
2	F	89	GLU	4.9
2	K	39	GLN	4.8
2	K	113	TRP	4.8
2	K	122	SER	4.7
2	E	111	ASP	4.7
2	J	14	ALA	4.7
2	J	10	GLY	4.7
2	F	53	PHE	4.6
2	F	113	TRP	4.6
2	E	79	VAL	4.6
2	F	72	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
2	K	95	TYR	4.6
2	K	2	VAL	4.6
2	J	35	GLY	4.5
2	J	68	PHE	4.5
2	E	83	MET	4.4
2	F	97	ALA	4.4
2	F	91	THR	4.4
2	F	44	GLU	4.4
2	F	39	GLN	4.4
2	F	10	GLY	4.3
2	J	123	SER	4.3
2	J	20	LEU	4.3
2	F	92	ALA	4.3
2	F	122	SER	4.2
2	F	73	ASP	4.2
2	J	122	SER	4.2
1	A	221	VAL	4.2
2	E	34	MET	4.2
2	E	42	GLY	4.1
2	F	12	VAL	4.1
2	K	44	GLU	4.0
2	E	86	LEU	4.0
2	F	35	GLY	4.0
2	F	40	LEU	4.0
2	E	11	LEU	4.0
2	J	94	TYR	3.9
2	J	13	GLN	3.9
2	E	94	TYR	3.9
2	K	91	THR	3.8
2	F	75	GLY	3.8
2	F	17	SER	3.8
2	E	71	SER	3.8
2	K	3	GLN	3.8
2	F	107	ARG	3.8
2	J	18	LEU	3.8
1	A	260	SER	3.7
2	F	84	ASN	3.7
2	K	4	LEU	3.7
2	F	7	SER	3.7
2	F	74	SER	3.7
2	K	10	GLY	3.6
2	F	51	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	K	111	ASP	3.6
2	F	68	PHE	3.6
2	F	38	ARG	3.6
2	F	5	GLN	3.6
2	K	88	PRO	3.6
1	C	267	TRP	3.5
2	L	76	LYS	3.5
2	E	75	GLY	3.5
2	L	42	GLY	3.5
2	K	16	GLY	3.5
2	F	87	LYS	3.5
2	K	5	GLN	3.5
2	J	8	GLY	3.5
2	E	96	CYS	3.5
1	C	266	ALA	3.5
2	J	86	LEU	3.5
1	C	258	ASN	3.4
2	E	122	SER	3.4
2	E	51	LEU	3.4
2	E	112	GLY	3.4
2	J	16	GLY	3.4
2	K	97	ALA	3.4
2	K	26	ARG	3.4
2	F	45	PRO	3.4
2	E	15	GLY	3.4
2	D	18	LEU	3.3
1	A	259	GLY	3.3
2	F	3	GLN	3.3
2	L	11	LEU	3.3
2	F	42	GLY	3.3
2	K	13	GLN	3.3
2	E	3	GLN	3.3
1	A	246	ALA	3.3
2	J	15	GLY	3.2
1	B	258	ASN	3.2
2	E	12	VAL	3.2
2	J	121	VAL	3.1
1	C	207	TRP	3.1
2	E	105	SER	3.1
2	K	24	ALA	3.1
2	E	121	VAL	3.1
1	A	51	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	37	PHE	3.1
2	E	20	LEU	3.1
2	K	92	ALA	3.0
2	E	95	TYR	3.0
2	E	88	PRO	3.0
2	E	41	ALA	3.0
2	F	86	LEU	3.0
2	F	117	THR	3.0
2	K	42	GLY	3.0
2	D	123	SER	3.0
2	E	28	THR	3.0
2	F	90	ASP	3.0
2	K	121	VAL	3.0
1	H	27	TYR	3.0
1	B	51	LEU	3.0
2	E	97	ALA	3.0
2	J	40	LEU	3.0
2	F	19	ARG	3.0
2	J	19	ARG	2.9
2	E	120	THR	2.9
2	J	85	SER	2.9
2	J	88	PRO	2.9
2	F	43	LYS	2.9
2	E	40	LEU	2.9
2	J	117	THR	2.9
2	E	26	ARG	2.9
2	F	26	ARG	2.9
2	L	122	SER	2.9
2	K	23	THR	2.9
2	K	98	ALA	2.9
2	F	93	ILE	2.9
1	B	221	VAL	2.8
2	E	80	TYR	2.8
2	E	44	GLU	2.8
2	F	67	ARG	2.8
2	E	90	ASP	2.8
2	K	93	ILE	2.8
1	A	267	TRP	2.8
3	Q	120	LYS	2.8
2	E	32	TRP	2.8
2	F	94	TYR	2.7
2	J	119	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	48	VAL	2.7
2	L	121	VAL	2.7
1	G	267	TRP	2.7
2	F	20	LEU	2.7
2	F	114	GLY	2.7
2	K	115	GLN	2.7
2	D	10	GLY	2.7
1	G	259	GLY	2.7
2	E	33	CYS	2.6
2	E	89	GLU	2.6
1	A	47	LEU	2.6
2	E	81	LEU	2.6
2	J	50	ALA	2.6
2	K	120	THR	2.6
2	E	113	TRP	2.6
2	L	10	GLY	2.6
2	F	120	THR	2.6
1	C	26	LEU	2.6
1	B	27	TYR	2.6
1	A	219	SER	2.6
2	E	114	GLY	2.6
2	L	91	THR	2.6
2	J	84	ASN	2.5
2	E	74	SER	2.5
2	E	9	GLY	2.5
2	K	119	VAL	2.5
1	B	23	ASP	2.5
2	K	43	LYS	2.5
1	A	201	TRP	2.5
2	E	108	GLU	2.5
2	F	25	SER	2.5
2	F	110	TYR	2.5
1	B	64	GLY	2.5
1	A	266	ALA	2.5
2	J	108	GLU	2.5
1	I	27	TYR	2.5
2	J	113	TRP	2.5
1	B	260	SER	2.4
2	D	17	SER	2.4
2	L	75	GLY	2.4
2	K	107	ARG	2.4
2	E	85	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	90	ASP	2.4
2	F	80	TYR	2.4
2	E	4	LEU	2.4
2	E	2	VAL	2.4
1	I	259	GLY	2.4
1	B	26	LEU	2.4
2	J	97	ALA	2.4
1	A	7	THR	2.4
1	B	219	SER	2.4
2	F	77	ASN	2.4
2	J	38	ARG	2.4
2	L	40	LEU	2.4
2	L	88	PRO	2.4
1	A	132	GLY	2.4
2	D	14	ALA	2.4
2	E	101	GLY	2.4
2	K	85	SER	2.4
2	D	76	LYS	2.4
2	J	42	GLY	2.4
1	A	53	VAL	2.4
2	L	24	ALA	2.4
2	J	44	GLU	2.3
1	H	30	LEU	2.3
2	L	44	GLU	2.3
2	J	93	ILE	2.3
1	H	26	LEU	2.3
2	J	48	VAL	2.3
2	L	120	THR	2.3
2	J	81	LEU	2.3
1	G	260	SER	2.3
2	K	11	LEU	2.3
2	J	17	SER	2.3
1	G	258	ASN	2.3
1	A	27	TYR	2.3
2	E	21	SER	2.3
2	F	63	SER	2.3
2	K	116	GLY	2.3
1	G	26	LEU	2.2
2	E	29	GLY	2.2
2	F	8	GLY	2.2
2	E	46	GLU	2.2
2	F	62	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	K	37	PHE	2.2
2	F	83	MET	2.2
1	C	30	LEU	2.2
2	J	90	ASP	2.2
1	A	52	ASN	2.2
1	B	259	GLY	2.2
2	L	108	GLU	2.2
2	E	37	PHE	2.2
2	K	45	PRO	2.2
1	A	74	VAL	2.2
2	J	87	LYS	2.1
2	L	123	SER	2.1
1	A	118	VAL	2.1
2	J	115	GLN	2.1
2	K	34	MET	2.1
2	K	117	THR	2.1
1	H	253	ILE	2.1
2	K	14	ALA	2.1
1	B	24	GLY	2.1
2	J	83	MET	2.1
2	E	76	LYS	2.1
2	F	56	ASP	2.1
2	E	8	GLY	2.1
2	J	2	VAL	2.1
2	L	9	GLY	2.1
1	B	66	TYR	2.1
1	C	220	LEU	2.1
2	J	116	GLY	2.1
2	J	39	GLN	2.1
2	E	73	ASP	2.1
1	I	31	THR	2.0
2	E	69	THR	2.0
2	J	49	VAL	2.0
1	A	50	ALA	2.0
1	B	30	LEU	2.0
2	F	118	GLN	2.0
2	L	113	TRP	2.0
2	J	61	ALA	2.0
1	C	259	GLY	2.0
1	C	260	SER	2.0
2	F	4	LEU	2.0
2	D	12	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	78	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.