



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:28 PM GMT

PDB ID : 1FRS
Title : CRYSTAL STRUCTURE OF BACTERIOPHAGE FR CAPSIDS AT 3.5
ANGSTROMS RESOLUTION
Authors : Liljas, L.; Valegard, K.; Bundule, M.
Deposited on : 1994-08-16
Resolution : 3.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

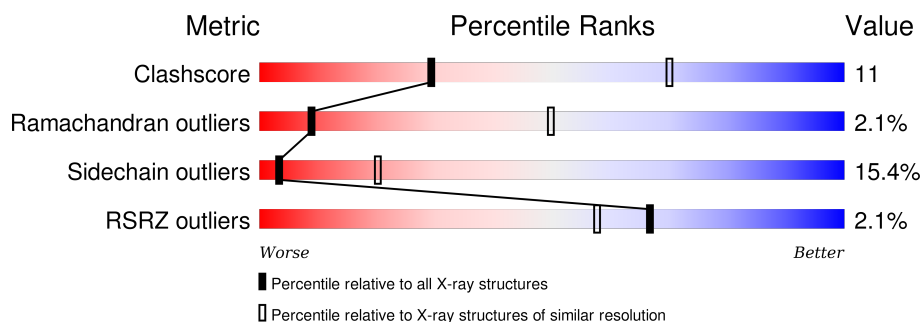
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 $\leq 5\%$. 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	129	<div> <div>2%</div> <div>50% 32% 16%</div> <div>.</div> </div>
1	B	129	<div> <div>%</div> <div>52% 35% 12%</div> <div>.</div> </div>
1	C	129	<div> <div>4%</div> <div>50% 36% 13%</div> <div>.</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2898 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.

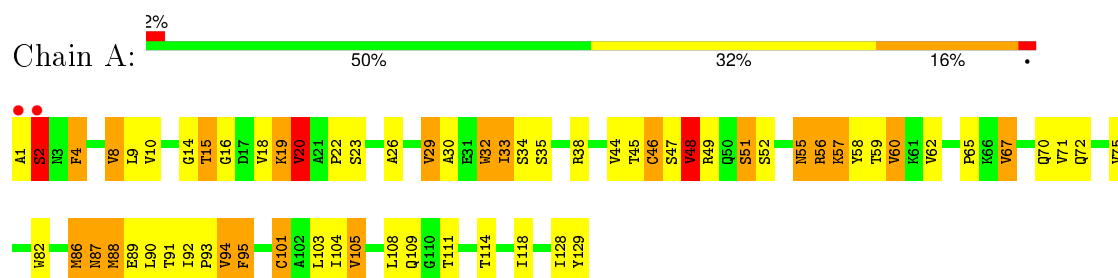
- Molecule 1 is a protein called BACTERIOPHAGE FR CAPSID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			966	606	166	190	4			
1	B	129	Total	C	N	O	S	0	0	0
			966	606	166	190	4			
1	C	129	Total	C	N	O	S	0	0	0
			966	606	166	190	4			

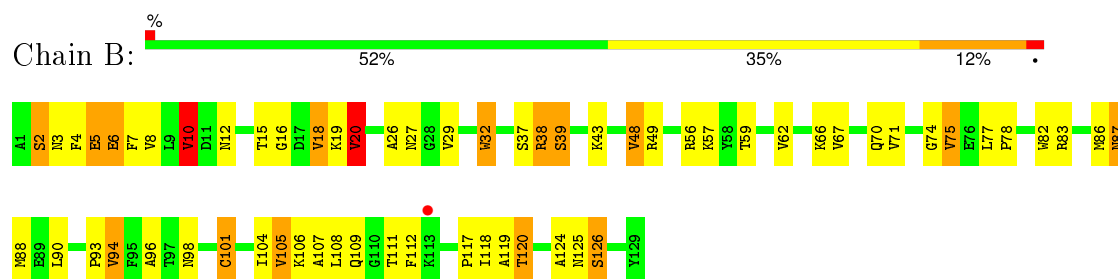
3 Residue-property plots [i](#)

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.

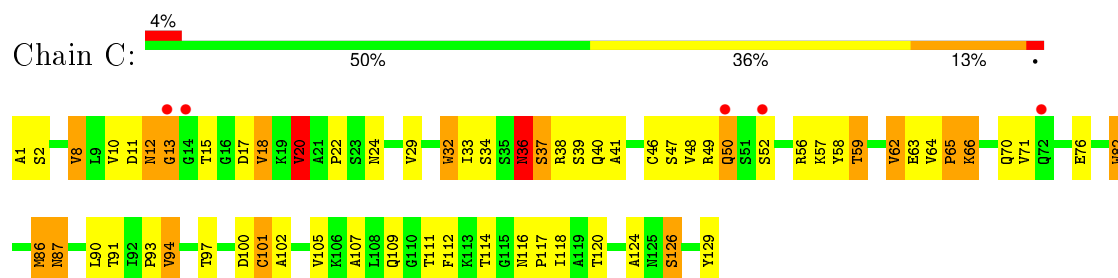
• Molecule 1: BACTERIOPHAGE FR CAPSID



• Molecule 1: BACTERIOPHAGE FR CAPSID



• Molecule 1: BACTERIOPHAGE FR CAPSID



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	422.90Å 305.90Å 274.80Å 90.00° 129.80° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 18.96 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.50) 28.1 (18.96-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.28Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.228 , 0.236 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.031 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 136356 reflections	Xtriage
F_o, F_c correlation	0.29	EDS
Total number of atoms	2898	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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, 0.375 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	1.66	11/983 (1.1%)	2.01	32/1337 (2.4%)
1	B	1.58	8/983 (0.8%)	2.10	42/1337 (3.1%)
1	C	1.60	7/983 (0.7%)	2.07	38/1337 (2.8%)
All	All	1.61	26/2949 (0.9%)	2.06	112/4011 (2.8%)

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	C	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	47	SER	CA-CB	-10.56	1.37	1.52
1	C	49	ARG	NE-CZ	8.54	1.44	1.33
1	A	49	ARG	CZ-NH2	8.04	1.43	1.33
1	A	49	ARG	NE-CZ	7.63	1.43	1.33
1	A	49	ARG	CZ-NH1	6.92	1.42	1.33
1	A	46	CYS	CA-CB	-6.68	1.39	1.53
1	C	49	ARG	CZ-NH2	6.31	1.41	1.33
1	A	89	GLU	CA-CB	-6.26	1.40	1.53
1	A	105	VAL	CA-CB	-6.05	1.42	1.54
1	B	49	ARG	CZ-NH2	6.04	1.41	1.33
1	B	49	ARG	CZ-NH1	5.93	1.40	1.33
1	B	105	VAL	CA-CB	-5.92	1.42	1.54
1	B	8	VAL	CA-CB	-5.86	1.42	1.54
1	C	62	VAL	CA-CB	-5.54	1.43	1.54
1	C	82	TRP	CG-CD2	-5.36	1.34	1.43
1	A	57	LYS	CA-CB	-5.28	1.42	1.53
1	A	95	PHE	CA-CB	-5.28	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	49	ARG	CG-CD	5.25	1.65	1.51
1	C	29	VAL	CA-CB	-5.21	1.43	1.54
1	A	32	TRP	CA-CB	-5.18	1.42	1.53
1	B	78	PRO	CA-CB	-5.17	1.43	1.53
1	B	49	ARG	NE-CZ	5.14	1.39	1.33
1	A	32	TRP	CG-CD2	-5.13	1.34	1.43
1	B	32	TRP	CG-CD2	-5.10	1.34	1.43
1	A	29	VAL	CA-CB	-5.09	1.44	1.54
1	B	32	TRP	CA-CB	-5.01	1.43	1.53

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	ARG	NE-CZ-NH2	-12.99	113.81	120.30
1	B	56	ARG	NE-CZ-NH2	-10.89	114.85	120.30
1	C	12	ASN	CA-C-N	-10.60	95.00	116.20
1	A	56	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	C	32	TRP	CD1-CG-CD2	9.93	114.25	106.30
1	A	32	TRP	CD1-CG-CD2	9.88	114.20	106.30
1	B	32	TRP	CD1-CG-CD2	9.44	113.85	106.30
1	B	48	VAL	CB-CA-C	-9.23	93.87	111.40
1	A	32	TRP	CE2-CD2-CG	-8.78	100.28	107.30
1	C	32	TRP	CE2-CD2-CG	-8.57	100.45	107.30
1	A	101	CYS	CA-CB-SG	-8.32	99.02	114.00
1	A	48	VAL	CB-CA-C	-8.26	95.71	111.40
1	C	101	CYS	CA-CB-SG	-8.18	99.28	114.00
1	A	82	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	B	32	TRP	CE2-CD2-CG	-7.94	100.94	107.30
1	A	82	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	B	10	VAL	CA-CB-CG2	-7.81	99.18	110.90
1	B	2	SER	N-CA-C	-7.58	90.53	111.00
1	B	94	VAL	CG1-CB-CG2	-7.29	99.24	110.90
1	A	46	CYS	CA-CB-SG	-7.07	101.28	114.00
1	A	2	SER	N-CA-C	-7.00	92.09	111.00
1	B	82	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	A	88	MET	CG-SD-CE	-6.97	89.05	100.20
1	B	82	TRP	CD1-CG-CD2	6.96	111.86	106.30
1	C	82	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	B	18	VAL	CA-C-N	-6.93	101.94	117.20
1	C	56	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	32	TRP	CB-CG-CD1	-6.88	118.06	127.00
1	B	108	LEU	CB-CA-C	-6.73	97.41	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	32	TRP	CG-CD2-CE3	6.65	139.88	133.90
1	C	32	TRP	CB-CG-CD1	-6.62	118.40	127.00
1	B	66	LYS	N-CA-C	-6.54	93.34	111.00
1	C	87	ASN	N-CA-CB	-6.54	98.83	110.60
1	B	15	THR	N-CA-CB	-6.46	98.03	110.30
1	B	101	CYS	CA-CB-SG	-6.41	102.46	114.00
1	A	44	VAL	CA-CB-CG2	-6.31	101.43	110.90
1	A	20	VAL	N-CA-CB	-6.29	97.66	111.50
1	C	36	ASN	CA-CB-CG	-6.27	99.61	113.40
1	B	62	VAL	CA-CB-CG1	-6.27	101.50	110.90
1	A	16	GLY	CA-C-N	-6.24	103.47	117.20
1	B	29	VAL	CA-CB-CG2	-6.21	101.59	110.90
1	A	44	VAL	CG1-CB-CG2	-6.21	100.97	110.90
1	C	82	TRP	CD1-CG-CD2	6.21	111.27	106.30
1	C	18	VAL	CA-CB-CG1	-6.18	101.63	110.90
1	C	18	VAL	CA-C-N	-6.17	103.63	117.20
1	A	1	ALA	CA-C-N	-6.16	103.64	117.20
1	C	8	VAL	CB-CA-C	-6.15	99.71	111.40
1	C	50	GLN	CA-C-N	6.12	130.68	117.20
1	B	5	GLU	CB-CA-C	-6.11	98.17	110.40
1	A	32	TRP	CG-CD2-CE3	6.09	139.38	133.90
1	A	1	ALA	O-C-N	6.08	132.43	122.70
1	C	32	TRP	CG-CD1-NE1	-6.06	104.04	110.10
1	A	82	TRP	CB-CG-CD1	-6.05	119.13	127.00
1	C	12	ASN	O-C-N	6.01	133.42	123.20
1	C	20	VAL	CA-CB-CG2	-6.00	101.90	110.90
1	C	2	SER	CA-C-N	-5.94	104.14	117.20
1	A	94	VAL	CG1-CB-CG2	-5.90	101.46	110.90
1	C	17	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	B	78	PRO	N-CD-CG	-5.83	94.46	103.20
1	B	75	VAL	N-CA-C	-5.83	95.27	111.00
1	A	15	THR	CA-CB-CG2	-5.82	104.25	112.40
1	B	20	VAL	N-CA-CB	-5.82	98.70	111.50
1	A	111	THR	CA-C-N	-5.80	104.45	117.20
1	B	83	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	94	VAL	N-CA-CB	-5.76	98.83	111.50
1	B	32	TRP	CB-CG-CD1	-5.74	119.54	127.00
1	B	32	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	C	49	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	C	86	MET	CA-C-N	-5.66	104.74	117.20
1	B	126	SER	O-C-N	5.66	132.82	123.20
1	B	10	VAL	CA-CB-CG1	5.62	119.33	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	C	20	VAL	N-CA-CB	-5.61	99.16	111.50
1	B	32	TRP	CG-CD2-CE3	5.61	138.94	133.90
1	C	118	ILE	CA-C-N	-5.60	104.87	117.20
1	C	86	MET	N-CA-C	-5.57	95.96	111.00
1	C	129	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	A	118	ILE	CA-C-N	-5.54	105.01	117.20
1	B	96	ALA	CA-C-N	-5.52	105.06	117.20
1	A	20	VAL	CA-CB-CG2	-5.50	102.64	110.90
1	A	87	ASN	N-CA-CB	-5.49	100.71	110.60
1	A	9	LEU	CB-CG-CD2	-5.48	101.69	111.00
1	B	87	ASN	CA-CB-CG	-5.48	101.34	113.40
1	B	74	GLY	CA-C-N	-5.45	105.21	117.20
1	B	83	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	15	THR	OG1-CB-CG2	5.44	122.52	110.00
1	A	38	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	37	SER	CA-C-N	-5.38	105.35	117.20
1	B	118	ILE	CA-C-N	-5.36	105.42	117.20
1	C	11	ASP	CA-C-N	-5.33	105.48	117.20
1	B	48	VAL	N-CA-CB	5.32	123.20	111.50
1	B	38	ARG	CA-CB-CG	-5.30	101.73	113.40
1	C	71	VAL	CA-CB-CG1	-5.29	102.96	110.90
1	B	43	LYS	CA-CB-CG	5.27	125.00	113.40
1	A	51	SER	N-CA-C	5.27	125.22	111.00
1	B	6	GLU	N-CA-CB	-5.24	101.17	110.60
1	C	58	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	B	108	LEU	N-CA-CB	5.21	120.82	110.40
1	B	71	VAL	CA-CB-CG1	-5.20	103.11	110.90
1	C	12	ASN	N-CA-C	-5.19	96.99	111.00
1	C	49	ARG	CA-CB-CG	5.19	124.81	113.40
1	C	94	VAL	CA-CB-CG2	-5.16	103.15	110.90
1	B	82	TRP	CA-C-N	5.16	128.56	117.20
1	A	82	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	A	128	ILE	CA-CB-CG1	-5.13	101.26	111.00
1	B	37	SER	N-CA-C	-5.13	97.16	111.00
1	B	8	VAL	O-C-N	5.09	130.84	122.70
1	C	117	PRO	N-CD-CG	-5.05	95.62	103.20
1	B	106	LYS	CG-CD-CE	5.05	127.05	111.90
1	C	112	PHE	CB-CG-CD2	-5.04	117.27	120.80
1	A	67	VAL	CB-CA-C	-5.03	101.84	111.40
1	C	109	GLN	CA-C-N	-5.03	106.15	116.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	116	ASN	Peptide

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	966	0	957	26	0
1	B	966	0	957	23	0
1	C	966	0	957	22	0
All	All	2898	0	2871	65	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 11.

All (65) 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:C:124:ALA:HB3	1:C:126:SER:HB2	1.64	0.79
1:B:20:VAL:HG13	1:B:32:TRP:HB3	1.65	0.77
1:A:23:SER:HB3	1:A:33:ILE:HD12	1.70	0.73
1:C:10:VAL:HB	1:C:18:VAL:HB	1.76	0.67
1:C:20:VAL:HG13	1:C:32:TRP:HB3	1.78	0.65
1:B:10:VAL:HB	1:B:18:VAL:CG2	2.28	0.64
1:A:95:PHE:HA	1:B:39:SER:OG	1.98	0.64
1:B:86:MET:SD	1:B:87:ASN:N	2.72	0.63
1:C:33:ILE:HG22	1:C:34:SER:O	1.99	0.62
1:B:10:VAL:HB	1:B:18:VAL:HG22	1.82	0.62
1:B:107:ALA:O	1:B:111:THR:HG23	2.01	0.61
1:A:86:MET:SD	1:A:87:ASN:N	2.74	0.60
1:C:107:ALA:O	1:C:111:THR:HG23	2.02	0.59
1:A:101:CYS:O	1:A:104:ILE:HB	2.03	0.59
1:A:46:CYS:SG	1:A:47:SER:N	2.76	0.57
1:A:8:VAL:HA	1:A:19:LYS:HA	1.85	0.57
1:A:57:LYS:HA	1:A:90:LEU:O	2.06	0.56
1:A:30:ALA:O	1:A:45:THR:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HB	1:A:18:VAL:HB	1.88	0.56
1:A:105:VAL:O	1:A:109:GLN:HG3	2.06	0.55
1:B:94:VAL:HG12	1:C:39:SER:HB3	1.88	0.54
1:A:62:VAL:HB	1:A:86:MET:HB3	1.90	0.54
1:C:13:GLY:O	1:C:15:THR:HG22	2.09	0.52
1:A:20:VAL:HG13	1:A:32:TRP:HB3	1.92	0.51
1:B:67:VAL:O	1:B:70:GLN:HB2	2.12	0.50
1:A:70:GLN:HG2	1:A:72:GLN:HG3	1.94	0.50
1:B:101:CYS:O	1:B:105:VAL:HG23	2.12	0.49
1:A:129:TYR:CD1	1:A:129:TYR:N	2.81	0.49
1:A:4:PHE:O	1:C:1:ALA:N	2.44	0.48
1:A:33:ILE:HG12	1:A:34:SER:O	2.12	0.48
1:A:71:VAL:HA	1:A:75:VAL:O	2.14	0.47
1:C:41:ALA:O	1:C:65:PRO:HG3	2.14	0.47
1:B:98:ASN:OD1	1:C:36:ASN:HA	2.16	0.46
1:B:6:GLU:HA	1:B:20:VAL:O	2.15	0.46
1:A:92:ILE:HG22	1:A:93:PRO:O	2.15	0.46
1:C:66:LYS:HG3	1:C:82:TRP:CZ2	2.51	0.46
1:C:102:ALA:O	1:C:105:VAL:HB	2.15	0.46
1:C:97:THR:O	1:C:100:ASP:HB2	2.16	0.46
1:C:46:CYS:HA	1:C:59:THR:O	2.17	0.45
1:B:124:ALA:O	1:B:125:ASN:HB2	2.17	0.45
1:B:3:ASN:O	1:B:5:GLU:N	2.50	0.45
1:A:95:PHE:HA	1:B:39:SER:HG	1.82	0.45
1:C:10:VAL:HB	1:C:18:VAL:CB	2.45	0.44
1:A:22:PRO:HD3	1:A:32:TRP:CD1	2.53	0.44
1:A:52:SER:HB3	1:A:55:ASN:OD1	2.18	0.44
1:C:62:VAL:HG12	1:C:63:GLU:N	2.31	0.44
1:A:56:ARG:O	1:A:91:THR:HA	2.18	0.44
1:B:26:ALA:O	1:B:27:ASN:HB2	2.17	0.43
1:C:70:GLN:O	1:C:76:GLU:HA	2.19	0.43
1:B:112:PHE:O	1:B:119:ALA:HB2	2.19	0.43
1:C:64:VAL:HA	1:C:65:PRO:HD3	1.83	0.43
1:B:105:VAL:O	1:B:109:GLN:HG3	2.19	0.43
1:C:86:MET:SD	1:C:87:ASN:N	2.92	0.42
1:C:101:CYS:O	1:C:105:VAL:HG23	2.18	0.42
1:A:48:VAL:HG13	1:A:58:TYR:CD2	2.55	0.42
1:B:7:PHE:O	1:B:19:LYS:HA	2.20	0.42
1:A:94:VAL:HG13	1:B:38:ARG:HB3	2.00	0.42
1:B:57:LYS:HA	1:B:90:LEU:O	2.19	0.42
1:A:45:THR:O	1:A:60:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:CYS:O	1:B:104:ILE:HB	2.20	0.41
1:B:117:PRO:HA	1:B:120:THR:OG1	2.20	0.41
1:A:26:ALA:O	1:A:29:VAL:HG22	2.20	0.41
1:C:90:LEU:HD12	1:C:91:THR:H	1.85	0.41
1:C:57:LYS:HA	1:C:90:LEU:O	2.21	0.40
1:B:12:ASN:HB2	1:B:16:GLY:O	2.22	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	127/129 (98%)	111 (87%)	12 (9%)	4 (3%)	5	41
1	B	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	24	70
1	C	127/129 (98%)	113 (89%)	11 (9%)	3 (2%)	7	47
All	All	381/387 (98%)	340 (89%)	33 (9%)	8 (2%)	9	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	B	2	SER
1	C	13	GLY
1	A	2	SER
1	C	36	ASN
1	A	14	GLY
1	C	65	PRO
1	A	65	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	104/104 (100%)	86 (83%)	18 (17%)	2	14
1	B	104/104 (100%)	92 (88%)	12 (12%)	7	33
1	C	104/104 (100%)	86 (83%)	18 (17%)	2	14
All	All	312/312 (100%)	264 (85%)	48 (15%)	3	20

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	4	PHE
1	A	8	VAL
1	A	15	THR
1	A	19	LYS
1	A	20	VAL
1	A	33	ILE
1	A	35	SER
1	A	48	VAL
1	A	55	ASN
1	A	59	THR
1	A	60	VAL
1	A	67	VAL
1	A	86	MET
1	A	88	MET
1	A	103	LEU
1	A	108	LEU
1	A	114	THR
1	B	4	PHE
1	B	10	VAL
1	B	20	VAL
1	B	39	SER
1	B	48	VAL
1	B	59	THR
1	B	75	VAL
1	B	77	LEU

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Mol	Chain	Res	Type
1	B	88	MET
1	B	93	PRO
1	B	120	THR
1	B	126	SER
1	C	8	VAL
1	C	12	ASN
1	C	20	VAL
1	C	22	PRO
1	C	24	ASN
1	C	37	SER
1	C	38	ARG
1	C	40	GLN
1	C	48	VAL
1	C	50	GLN
1	C	52	SER
1	C	59	THR
1	C	66	LYS
1	C	93	PRO
1	C	94	VAL
1	C	114	THR
1	C	120	THR
1	C	126	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	ASN
1	C	40	GLN

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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	129/129 (100%)	0.43	2 (1%) 74 65	2, 21, 64, 88	0
1	B	129/129 (100%)	0.32	1 (0%) 87 80	3, 21, 55, 92	0
1	C	129/129 (100%)	0.42	5 (3%) 43 35	3, 21, 54, 83	0
All	All	387/387 (100%)	0.39	8 (2%) 67 58	2, 21, 61, 92	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14	GLY	3.9
1	A	1	ALA	2.8
1	C	52	SER	2.6
1	C	72	GLN	2.5
1	C	13	GLY	2.4
1	A	2	SER	2.3
1	C	50	GLN	2.2
1	B	113	LYS	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.