



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:10 AM UTC

PDB ID : 2X8K / pdb_00002x8k
Title : Crystal Structure of SPP1 Dit (gp 19.1) Protein, a Paradigm of Hub Adsorption Apparatus in Gram-positive Infecting Phages.
Authors : Veesler, D.; Robin, G.; Lichiere, J.; Auzat, I.; Tavares, P.; Bron, P.; Campanacci, V.; Cambillau, C.
Deposited on : 2010-03-10
Resolution : 2.95 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

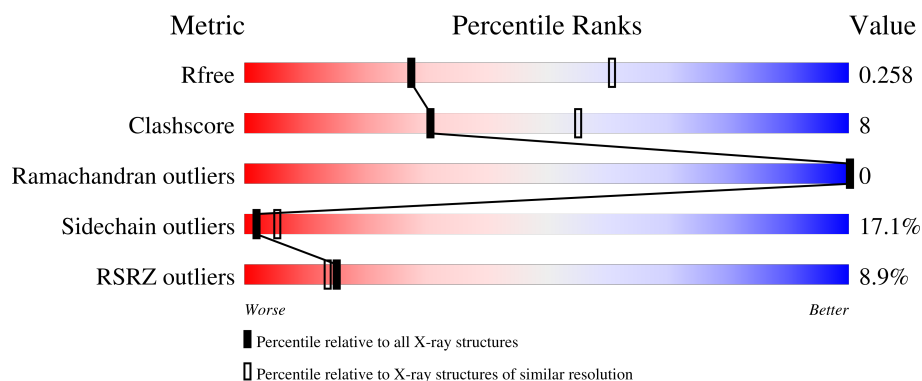
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	252	9% 70% 21% • • •
1	B	252	5% 71% 19% • • •
1	C	252	12% 66% 24% 5% • •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5710 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 HYPOTHETICAL PROTEIN 19.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1902	1210	306	378	8			
1	B	242	Total	C	N	O	S	0	0	0
			1902	1210	306	378	8			
1	C	243	Total	C	N	O	S	0	0	0
			1906	1212	307	379	8			

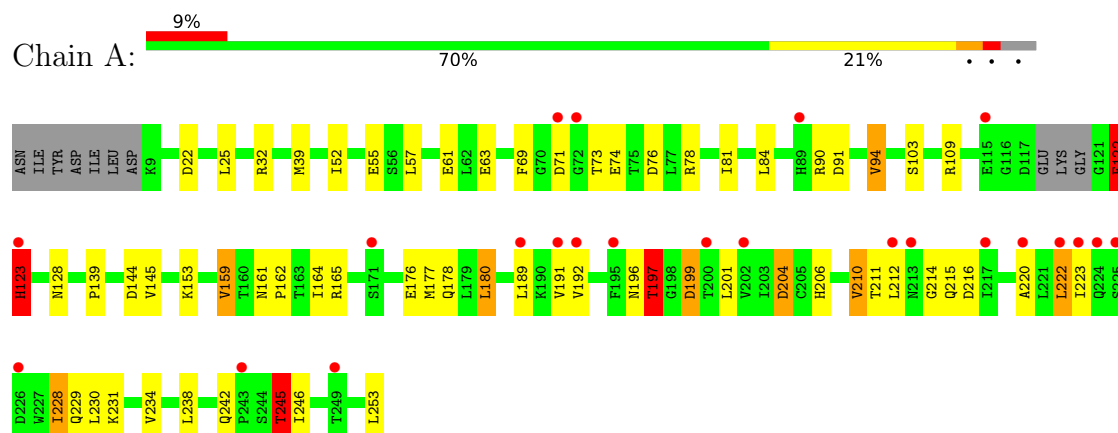
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	VAL	LYS	conflict	UNP O48459
B	192	VAL	LYS	conflict	UNP O48459
C	192	VAL	LYS	conflict	UNP O48459

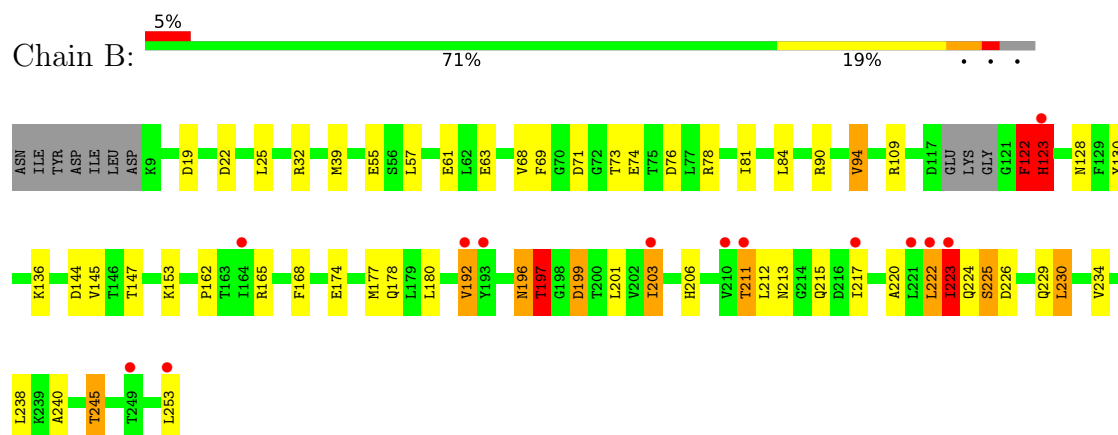
3 Residue-property plots [i](#)

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.

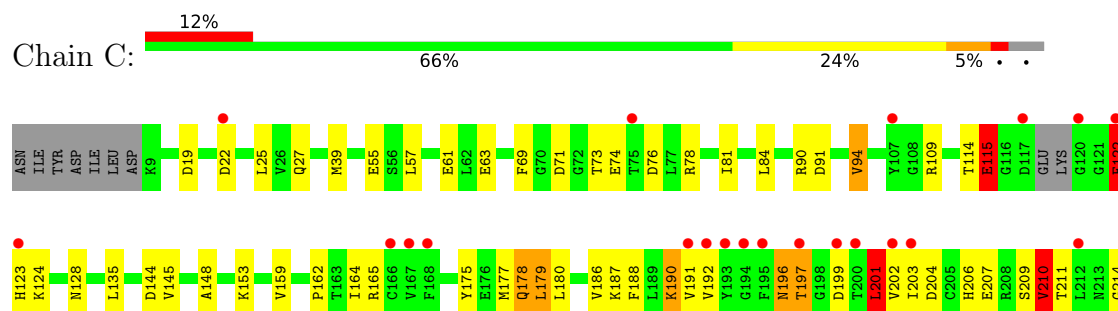
• Molecule 1: HYPOTHETICAL PROTEIN 19.1

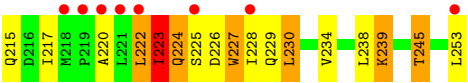


• Molecule 1: HYPOTHETICAL PROTEIN 19.1



• Molecule 1: HYPOTHETICAL PROTEIN 19.1





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	107.19Å 125.75Å 189.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.37 – 2.95 34.37 – 2.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.37-2.95) 99.3 (34.37-2.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.95Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.200 , 0.236 0.222 , 0.258	Depositor DCC
R_{free} test set	958 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å ²)	84.0	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5710	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.84	0/1940	1.38	20/2639 (0.8%)
1	B	0.80	0/1940	1.41	23/2639 (0.9%)
1	C	0.88	1/1944 (0.1%)	1.41	25/2644 (0.9%)
All	All	0.84	1/5824 (0.0%)	1.40	68/7922 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	202	VAL	CA-C	5.00	1.58	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ILE	N-CA-C	-16.65	85.32	108.96
1	A	223	ILE	N-CA-C	-14.94	87.75	108.96
1	B	222	LEU	N-CA-C	13.54	133.71	111.37
1	C	222	LEU	N-CA-C	12.72	132.36	111.37
1	C	223	ILE	N-CA-C	-11.32	85.80	109.34
1	A	222	LEU	N-CA-C	10.82	129.22	111.37
1	B	223	ILE	N-CA-CB	10.62	126.31	112.60
1	A	122	PHE	N-CA-C	9.18	120.02	108.45
1	A	223	ILE	N-CA-CB	8.26	123.26	112.60
1	A	94	VAL	N-CA-CB	-8.13	102.94	111.64
1	B	94	VAL	N-CA-CB	-7.99	103.09	111.64
1	B	222	LEU	CB-CA-C	-7.95	97.55	110.74
1	C	222	LEU	CB-CA-C	-7.90	97.62	110.74
1	C	94	VAL	N-CA-CB	-7.70	103.40	111.64
1	C	225	SER	CA-C-N	7.60	132.23	120.75
1	C	225	SER	C-N-CA	7.60	132.23	120.75
1	B	122	PHE	N-CA-C	7.58	119.55	108.86
1	A	197	THR	CB-CA-C	-7.16	102.74	109.83
1	B	197	THR	CB-CA-C	-7.07	102.83	109.83
1	C	225	SER	N-CA-C	-6.94	96.48	108.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	22	ASP	N-CA-C	-6.78	105.01	113.28
1	B	122	PHE	CA-C-N	6.64	132.96	122.34
1	B	122	PHE	C-N-CA	6.64	132.96	122.34
1	A	222	LEU	CB-CA-C	-6.45	100.03	110.74
1	B	22	ASP	N-CA-C	-6.42	105.45	113.28
1	C	226	ASP	N-CA-C	6.35	118.99	110.35
1	A	22	ASP	N-CA-C	-6.34	105.55	113.28
1	B	213	ASN	N-CA-C	6.15	125.59	113.29
1	C	223	ILE	N-CA-CB	6.14	121.37	111.23
1	C	122	PHE	CA-CB-CG	6.00	119.80	113.80
1	C	201	LEU	N-CA-C	5.99	118.69	108.02
1	A	69	PHE	CA-CB-CG	5.96	119.76	113.80
1	C	178	GLN	N-CA-C	5.91	118.36	108.73
1	B	22	ASP	CA-CB-CG	5.90	118.50	112.60
1	C	22	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	22	ASP	CA-CB-CG	5.80	118.40	112.60
1	B	69	PHE	CA-CB-CG	5.69	119.49	113.80
1	A	69	PHE	CA-C-N	5.61	125.67	120.34
1	A	69	PHE	C-N-CA	5.61	125.67	120.34
1	A	94	VAL	N-CA-C	5.60	113.78	109.19
1	C	224	GLN	CA-C-N	5.57	130.52	122.16
1	C	224	GLN	C-N-CA	5.57	130.52	122.16
1	C	94	VAL	CB-CA-C	5.54	114.76	109.33
1	C	19	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	94	VAL	CB-CA-C	5.40	114.63	109.33
1	C	115	GLU	N-CA-C	5.40	117.84	110.55
1	A	94	VAL	CB-CA-C	5.37	114.59	109.33
1	A	180	LEU	N-CA-C	5.33	117.18	109.07
1	A	245	THR	CB-CA-C	5.33	118.99	109.65
1	C	227	TRP	N-CA-C	-5.33	102.59	110.48
1	A	228	ILE	N-CA-C	5.31	115.84	110.05
1	B	123	HIS	N-CA-C	5.29	117.93	107.98
1	C	94	VAL	N-CA-C	5.25	113.50	109.19
1	A	123	HIS	N-CA-C	5.22	117.80	107.98
1	A	199	ASP	CA-CB-CG	5.22	117.82	112.60
1	C	69	PHE	CA-CB-CG	5.21	119.01	113.80
1	B	224	GLN	N-CA-C	-5.21	99.71	110.80
1	B	19	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	196	ASN	CA-CB-CG	5.18	117.78	112.60
1	B	199	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	135	LEU	N-CA-C	5.14	118.49	110.32
1	C	196	ASN	CA-CB-CG	5.13	117.73	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	GLN	CA-C-N	5.12	128.14	120.87
1	B	215	GLN	C-N-CA	5.12	128.14	120.87
1	A	216	ASP	N-CA-C	5.08	116.77	108.63
1	B	94	VAL	N-CA-C	5.08	113.35	109.19
1	C	210	VAL	N-CA-C	5.07	116.01	108.46
1	B	168	PHE	N-CA-C	5.01	117.60	110.24

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	1902	0	1847	27	0
1	B	1902	0	1847	20	0
1	C	1906	0	1850	47	0
All	All	5710	0	5544	93	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 8.

All (93) 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:187:LYS:CD	1:C:228:ILE:HG22	1.67	1.22
1:C:187:LYS:HD3	1:C:228:ILE:CG2	1.89	1.01
1:A:164:ILE:HD11	1:A:228:ILE:HD11	1.49	0.93
1:C:187:LYS:HD3	1:C:228:ILE:HG22	0.92	0.91
1:C:179:LEU:HD13	1:C:228:ILE:HD12	1.59	0.85
1:C:197:THR:O	1:C:197:THR:HG23	1.77	0.85
1:A:164:ILE:HD11	1:A:228:ILE:CD1	2.11	0.80
1:B:197:THR:O	1:B:197:THR:HG23	1.81	0.79
1:A:197:THR:HG23	1:A:197:THR:O	1.83	0.78
1:C:148:ALA:C	1:C:239:LYS:HG3	2.11	0.75
1:C:188:PHE:CE2	1:C:190:LYS:HD3	2.24	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LYS:CD	1:C:228:ILE:CG2	2.57	0.73
1:A:165:ARG:HB3	1:A:245:THR:HG22	1.74	0.69
1:C:177:MET:HE2	1:C:238:LEU:HB3	1.73	0.69
1:C:179:LEU:CD1	1:C:228:ILE:HD12	2.23	0.69
1:A:162:PRO:HD2	1:A:228:ILE:HG13	1.73	0.68
1:C:165:ARG:HB3	1:C:245:THR:HG22	1.76	0.68
1:B:165:ARG:HB3	1:B:245:THR:HG22	1.76	0.67
1:C:207:GLU:HA	1:C:227:TRP:CH2	2.30	0.67
1:B:177:MET:HE2	1:B:238:LEU:HB3	1.78	0.66
1:B:192:VAL:HG23	1:B:220:ALA:O	1.97	0.64
1:C:220:ALA:O	1:C:222:LEU:HD12	1.97	0.64
1:C:203:ILE:HG12	1:C:206:HIS:H	1.65	0.61
1:A:191:VAL:HG13	1:A:220:ALA:HB1	1.83	0.61
1:A:196:ASN:O	1:A:197:THR:HB	2.00	0.61
1:B:196:ASN:O	1:B:197:THR:HB	2.02	0.60
1:A:211:THR:HG23	1:A:212:LEU:N	2.17	0.58
1:B:145:VAL:HG11	1:B:177:MET:HE1	1.85	0.57
1:A:164:ILE:CD1	1:A:228:ILE:HD11	2.30	0.57
1:C:145:VAL:HG11	1:C:177:MET:HE1	1.87	0.56
1:C:179:LEU:HB2	1:C:228:ILE:HD13	1.87	0.55
1:C:196:ASN:O	1:C:197:THR:HB	2.05	0.55
1:C:165:ARG:HE	1:C:201:LEU:HD21	1.73	0.54
1:A:177:MET:HE2	1:A:238:LEU:HB3	1.90	0.54
1:C:207:GLU:HG2	1:C:227:TRP:CE2	2.43	0.53
1:C:191:VAL:HG22	1:C:220:ALA:HB1	1.90	0.53
1:C:207:GLU:HA	1:C:227:TRP:CZ3	2.44	0.53
1:A:145:VAL:HG11	1:A:177:MET:HE1	1.91	0.52
1:C:204:ASP:HA	1:C:227:TRP:CE3	2.44	0.52
1:B:211:THR:HB	1:B:217:ILE:HG13	1.91	0.52
1:C:179:LEU:HB2	1:C:228:ILE:CD1	2.40	0.51
1:A:162:PRO:HG3	1:A:230:LEU:HD13	1.93	0.50
1:A:162:PRO:HG2	1:A:228:ILE:HD12	1.94	0.49
1:C:148:ALA:CA	1:C:239:LYS:HG3	2.42	0.49
1:C:187:LYS:CB	1:C:228:ILE:CG2	2.90	0.49
1:C:204:ASP:OD2	1:C:227:TRP:HB3	2.12	0.49
1:A:122:PHE:CD1	1:A:122:PHE:N	2.79	0.49
1:A:210:VAL:HG13	1:A:214:GLY:HA2	1.95	0.49
1:C:179:LEU:HD23	1:C:186:VAL:HB	1.94	0.49
1:B:71:ASP:HB3	1:B:76:ASP:HB3	1.96	0.48
1:C:27:GLN:HE22	1:C:124:LYS:NZ	2.12	0.48
1:A:71:ASP:HB3	1:A:76:ASP:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLY:O	1:A:215:GLN:NE2	2.48	0.47
1:B:68:VAL:O	1:B:123:HIS:ND1	2.47	0.47
1:C:175:TYR:O	1:C:190:LYS:HA	2.16	0.46
1:C:71:ASP:HB3	1:C:76:ASP:HB3	1.97	0.46
1:B:203:ILE:HG12	1:B:206:HIS:H	1.79	0.46
1:C:187:LYS:HB2	1:C:228:ILE:HG21	1.97	0.46
1:A:196:ASN:O	1:A:197:THR:CB	2.65	0.45
1:B:147:THR:HA	1:B:240:ALA:O	2.16	0.45
1:C:187:LYS:HB3	1:C:228:ILE:CG2	2.47	0.44
1:C:115:GLU:HG3	1:C:123:HIS:CE1	2.52	0.44
1:C:162:PRO:HG3	1:C:230:LEU:HD13	1.99	0.44
1:B:196:ASN:O	1:B:197:THR:CB	2.65	0.44
1:C:187:LYS:CB	1:C:228:ILE:HG21	2.48	0.44
1:C:222:LEU:HD12	1:C:222:LEU:H	1.83	0.43
1:A:161:ASN:HB3	1:A:204:ASP:HB3	2.01	0.43
1:A:39:MET:HG2	1:A:55:GLU:HG3	2.01	0.43
1:B:39:MET:HG2	1:B:55:GLU:HG3	1.99	0.43
1:A:61:GLU:OE2	1:A:128:ASN:HB3	2.19	0.42
1:B:197:THR:O	1:B:197:THR:CG2	2.47	0.42
1:C:39:MET:HG2	1:C:55:GLU:HG3	2.00	0.42
1:C:196:ASN:O	1:C:197:THR:CB	2.67	0.42
1:C:223:ILE:HG22	1:C:224:GLN:N	2.34	0.42
1:C:207:GLU:CA	1:C:227:TRP:CH2	3.01	0.42
1:B:122:PHE:CD1	1:B:122:PHE:N	2.86	0.42
1:C:210:VAL:HG13	1:C:214:GLY:HA2	2.02	0.42
1:B:122:PHE:HB2	1:B:123:HIS:H	1.70	0.42
1:A:52:ILE:HD11	1:B:130:TYR:HD2	1.85	0.42
1:A:122:PHE:HB2	1:A:123:HIS:H	1.62	0.41
1:C:227:TRP:CD1	1:C:227:TRP:H	2.38	0.41
1:A:159:VAL:HG22	1:A:231:LYS:HA	2.03	0.41
1:C:122:PHE:HD1	1:C:122:PHE:C	2.29	0.41
1:B:61:GLU:OE2	1:B:128:ASN:HB3	2.20	0.41
1:A:103:SER:HB3	1:A:139:PRO:HG3	2.03	0.41
1:C:122:PHE:C	1:C:122:PHE:CD1	2.99	0.41
1:B:223:ILE:O	1:B:225:SER:N	2.54	0.41
1:C:187:LYS:HD2	1:C:228:ILE:HG22	1.84	0.41
1:C:188:PHE:HE2	1:C:190:LYS:HD3	1.77	0.41
1:A:176:GLU:HA	1:A:189:LEU:O	2.20	0.40
1:B:162:PRO:HG3	1:B:230:LEU:HD13	2.04	0.40
1:C:61:GLU:OE2	1:C:128:ASN:HB3	2.20	0.40
1:A:162:PRO:HG2	1:A:228:ILE:CD1	2.52	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	238/252 (94%)	220 (92%)	18 (8%)	0	100	100
1	B	238/252 (94%)	219 (92%)	19 (8%)	0	100	100
1	C	239/252 (95%)	220 (92%)	19 (8%)	0	100	100
All	All	715/756 (95%)	659 (92%)	56 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	212/225 (94%)	178 (84%)	34 (16%)	2	8
1	B	212/225 (94%)	176 (83%)	36 (17%)	2	5
1	C	212/225 (94%)	173 (82%)	39 (18%)	1	4
All	All	636/675 (94%)	527 (83%)	109 (17%)	2	5

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	32	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	57	LEU
1	A	63	GLU
1	A	73	THR
1	A	74	GLU
1	A	78	ARG
1	A	81	ILE
1	A	84	LEU
1	A	90	ARG
1	A	91	ASP
1	A	94	VAL
1	A	109	ARG
1	A	122	PHE
1	A	123	HIS
1	A	144	ASP
1	A	153	LYS
1	A	159	VAL
1	A	178	GLN
1	A	180	LEU
1	A	192	VAL
1	A	197	THR
1	A	199	ASP
1	A	201	LEU
1	A	204	ASP
1	A	206	HIS
1	A	210	VAL
1	A	222	LEU
1	A	229	GLN
1	A	234	VAL
1	A	242	GLN
1	A	245	THR
1	A	246	ILE
1	A	253	LEU
1	B	25	LEU
1	B	32	ARG
1	B	57	LEU
1	B	63	GLU
1	B	73	THR
1	B	74	GLU
1	B	78	ARG
1	B	81	ILE
1	B	84	LEU
1	B	90	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	94	VAL
1	B	109	ARG
1	B	122	PHE
1	B	123	HIS
1	B	136	LYS
1	B	144	ASP
1	B	153	LYS
1	B	174	GLU
1	B	178	GLN
1	B	180	LEU
1	B	192	VAL
1	B	197	THR
1	B	199	ASP
1	B	201	LEU
1	B	203	ILE
1	B	211	THR
1	B	212	LEU
1	B	222	LEU
1	B	223	ILE
1	B	225	SER
1	B	226	ASP
1	B	229	GLN
1	B	230	LEU
1	B	234	VAL
1	B	245	THR
1	B	253	LEU
1	C	25	LEU
1	C	57	LEU
1	C	63	GLU
1	C	73	THR
1	C	74	GLU
1	C	78	ARG
1	C	81	ILE
1	C	84	LEU
1	C	90	ARG
1	C	91	ASP
1	C	94	VAL
1	C	109	ARG
1	C	114	THR
1	C	115	GLU
1	C	122	PHE
1	C	144	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	153	LYS
1	C	159	VAL
1	C	164	ILE
1	C	178	GLN
1	C	179	LEU
1	C	180	LEU
1	C	190	LYS
1	C	192	VAL
1	C	197	THR
1	C	199	ASP
1	C	201	LEU
1	C	209	SER
1	C	210	VAL
1	C	211	THR
1	C	215	GLN
1	C	217	ILE
1	C	223	ILE
1	C	229	GLN
1	C	230	LEU
1	C	234	VAL
1	C	239	LYS
1	C	245	THR
1	C	253	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	178	GLN
1	B	229	GLN
1	C	27	GLN
1	C	123	HIS
1	C	128	ASN
1	C	224	GLN

5.3.3 RNA ⓘ

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	242/252 (96%)	0.70	23 (9%) 14 12	52, 107, 188, 202	0
1	B	242/252 (96%)	0.50	13 (5%) 31 26	57, 93, 171, 191	0
1	C	243/252 (96%)	0.68	29 (11%) 9 8	57, 98, 185, 194	0
All	All	727/756 (96%)	0.63	65 (8%) 15 14	52, 98, 184, 202	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	VAL	6.4
1	C	222	LEU	6.2
1	A	226	ASP	6.1
1	A	225	SER	4.7
1	C	191	VAL	4.0
1	C	167	VAL	3.8
1	C	228	ILE	3.7
1	B	222	LEU	3.7
1	C	225	SER	3.4
1	C	220	ALA	3.1
1	C	192	VAL	3.1
1	A	192	VAL	3.0
1	C	200	THR	3.0
1	C	203	ILE	3.0
1	C	120	GLY	2.9
1	C	107	TYR	2.8
1	B	193	TYR	2.8
1	C	212	LEU	2.8
1	C	166	CYS	2.8
1	A	217	ILE	2.8
1	C	168	PHE	2.7
1	C	253	LEU	2.7
1	A	171	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	253	LEU	2.6
1	C	221	LEU	2.6
1	A	249	THR	2.6
1	C	199	ASP	2.5
1	C	117	ASP	2.5
1	B	203	ILE	2.4
1	C	194	GLY	2.4
1	A	195	PHE	2.4
1	C	197	THR	2.4
1	B	223	ILE	2.4
1	B	192	VAL	2.4
1	C	219	PRO	2.4
1	C	218	MET	2.4
1	B	221	LEU	2.3
1	B	164	ILE	2.3
1	A	71	ASP	2.3
1	A	212	LEU	2.3
1	A	243	PRO	2.3
1	A	72	GLY	2.3
1	A	123	HIS	2.3
1	C	75	THR	2.3
1	A	224	GLN	2.2
1	A	200	THR	2.2
1	A	89	HIS	2.2
1	C	22	ASP	2.2
1	C	122	PHE	2.2
1	A	189	LEU	2.2
1	A	202	VAL	2.2
1	A	220	ALA	2.2
1	B	123	HIS	2.2
1	A	115	GLU	2.2
1	B	249	THR	2.1
1	B	210	VAL	2.1
1	B	211	THR	2.1
1	C	193	TYR	2.1
1	C	123	HIS	2.1
1	C	195	PHE	2.1
1	B	217	ILE	2.1
1	A	222	LEU	2.1
1	C	202	VAL	2.0
1	A	213	ASN	2.0
1	A	223	ILE	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.