



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:01 am GMT

PDB ID : 4C0Z
Title : The N-terminal domain of the Streptococcus pyogenes pilus tip adhesin Cpa
Authors : Linke-Winnebeck, C.; Paterson, N.; Baker, E.N.
Deposited on : 2013-08-08
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

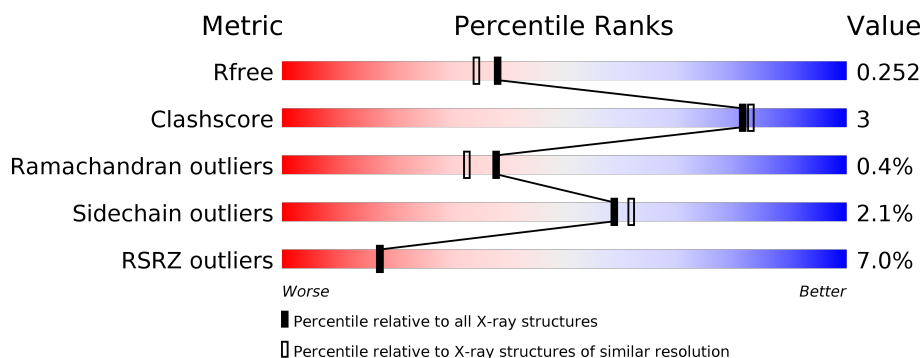
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	215	<div> <div style="width: 94%;"></div> <div>94%</div> </div>
1	B	215	<div> <div style="width: 91%;"></div> <div>91%</div> <div>5%</div> </div>
1	C	215	<div> <div style="width: 83%;"></div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
1	D	215	<div> <div style="width: 93%;"></div> <div>93%</div> </div>
1	E	215	<div> <div style="width: 91%;"></div> <div>91%</div> <div>5%</div> </div>
1	F	215	<div> <div style="width: 91%;"></div> <div>91%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	215	
1	H	215	
1	I	215	
1	J	215	
1	K	215	
1	L	215	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	B	1221	-	-	-	X
3	SPD	A	1223	-	-	-	X
3	SPD	G	1220	-	-	-	X
4	PO4	B	1220	-	-	-	X
4	PO4	F	1222	-	-	-	X
5	GOL	I	1220	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21588 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 ANCILLARY PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	2	0
			1718	1091	285	339	3			
1	B	208	Total	C	N	O	S	0	0	0
			1706	1084	284	335	3			
1	C	205	Total	C	N	O	S	0	3	0
			1710	1090	283	334	3			
1	D	208	Total	C	N	O	S	0	2	0
			1718	1091	285	339	3			
1	E	206	Total	C	N	O	S	0	1	0
			1700	1081	282	334	3			
1	F	209	Total	C	N	O	S	0	1	0
			1722	1094	286	339	3			
1	G	207	Total	C	N	O	S	0	1	0
			1701	1082	282	334	3			
1	H	208	Total	C	N	O	S	0	2	0
			1716	1091	284	338	3			
1	I	207	Total	C	N	O	S	0	1	0
			1703	1082	283	335	3			
1	J	207	Total	C	N	O	S	0	2	0
			1700	1082	280	335	3			
1	K	206	Total	C	N	O	S	0	0	0
			1680	1068	277	332	3			
1	L	209	Total	C	N	O	S	0	1	0
			1722	1094	286	339	3			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

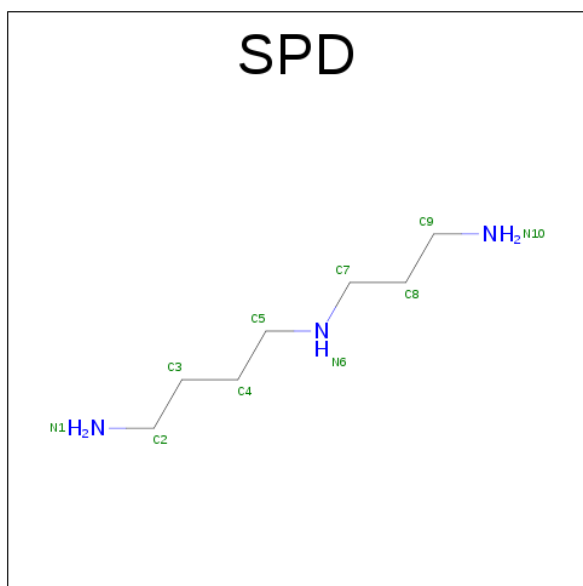
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Cl	0	0
			1	1		
2	J	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Cl	0	0
			1	1		
2	H	3	Total	Cl	0	0
			3	3		
2	B	2	Total	Cl	0	0
			2	2		
2	C	1	Total	Cl	0	0
			1	1		
2	A	2	Total	Cl	0	0
			2	2		
2	L	2	Total	Cl	0	0
			2	2		
2	F	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



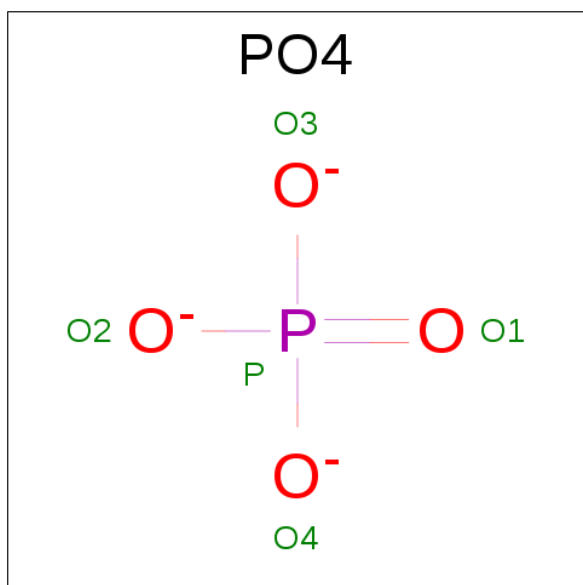
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	7	3		
3	C	1	Total	C	N	0	0
			10	7	3		
3	F	1	Total	C	N	0	0
			10	7	3		
3	G	1	Total	C	N	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	C	N	0	0
			10	7	3		
3	L	1	Total	C	N	0	0
			10	7	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	108	Total	O	0	0
			108	108		
6	B	73	Total	O	0	0
			73	73		
6	C	117	Total	O	0	0
			117	117		
6	D	93	Total	O	0	0
			93	93		
6	E	79	Total	O	0	0
			79	79		
6	F	79	Total	O	0	0
			79	79		
6	G	93	Total	O	0	0
			93	93		
6	H	69	Total	O	0	0
			69	69		
6	I	66	Total	O	0	0
			66	66		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	83	Total 83	O 83	0	0
6	K	58	Total 58	O 58	0	0
6	L	67	Total 67	O 67	0	0

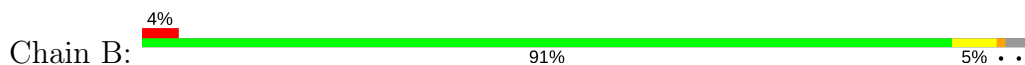
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

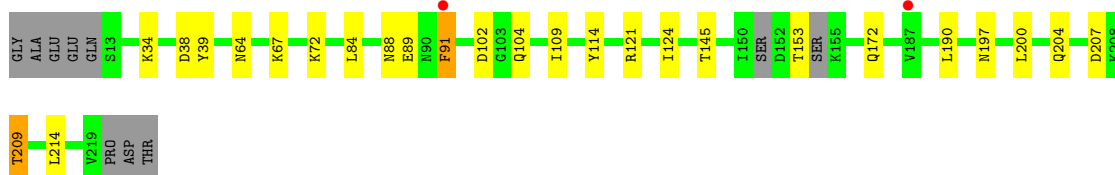
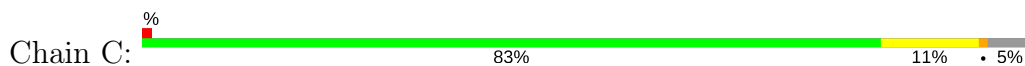
- Molecule 1: ANCILLARY PROTEIN 2



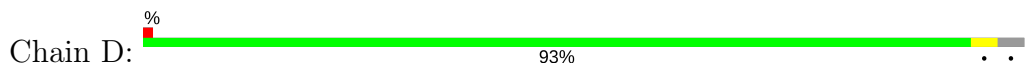
- Molecule 1: ANCILLARY PROTEIN 2



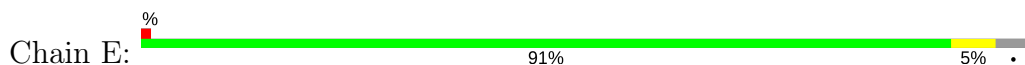
- Molecule 1: ANCILLARY PROTEIN 2



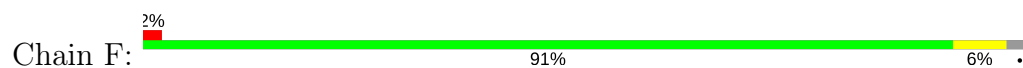
- Molecule 1: ANCILLARY PROTEIN 2



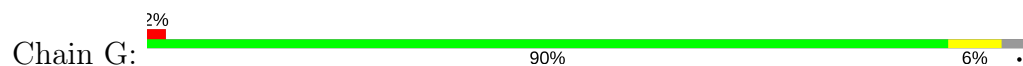
- Molecule 1: ANCILLARY PROTEIN 2



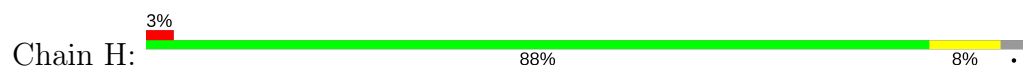
- Molecule 1: ANCILLARY PROTEIN 2



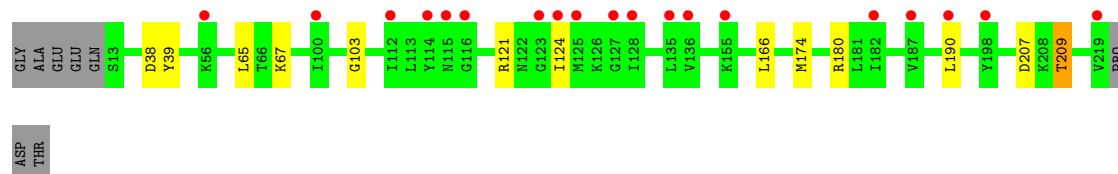
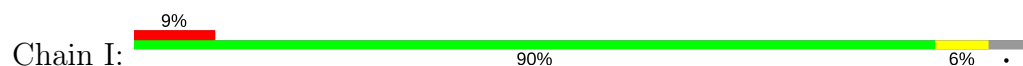
- Molecule 1: ANCILLARY PROTEIN 2



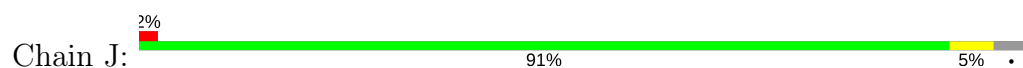
- Molecule 1: ANCILLARY PROTEIN 2



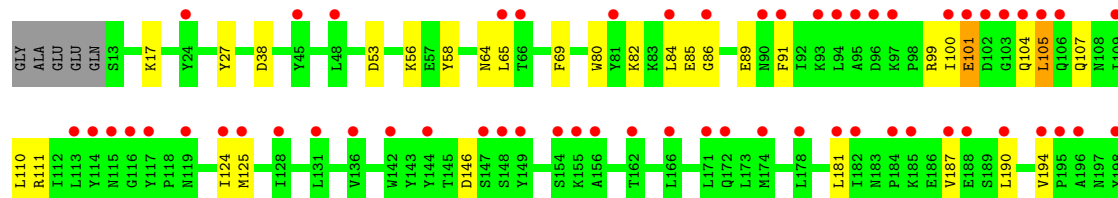
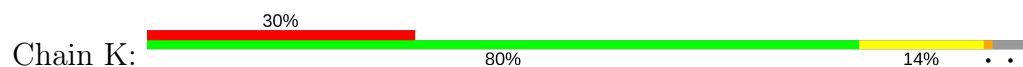
- Molecule 1: ANCILLARY PROTEIN 2

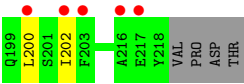


- Molecule 1: ANCILLARY PROTEIN 2

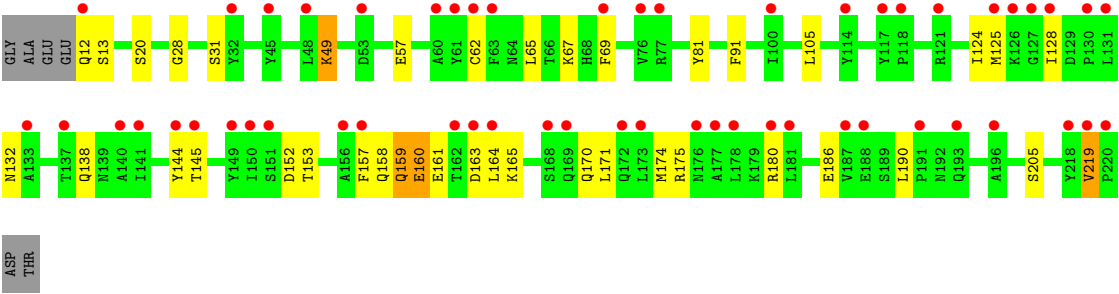
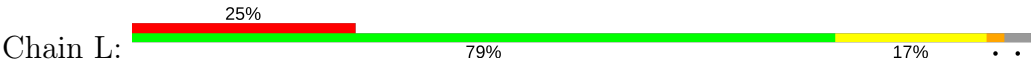


- Molecule 1: ANCILLARY PROTEIN 2





● Molecule 1: ANCILLARY PROTEIN 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	132.22Å 132.22Å 136.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.50 – 2.00 47.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.50-2.00) 99.6 (47.50-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.201 , 0.232 0.214 , 0.252	Depositor DCC
R_{free} test set	9226 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l 0.031 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21588	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.09 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1526e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, SPD, CL

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	0.48	0/1760	0.61	0/2387
1	B	0.48	0/1747	0.62	0/2368
1	C	0.51	0/1753	0.64	0/2373
1	D	0.49	0/1760	0.62	0/2387
1	E	0.48	0/1741	0.64	0/2360
1	F	0.48	0/1764	0.62	0/2392
1	G	0.46	0/1745	0.62	0/2366
1	H	0.47	0/1761	0.63	0/2388
1	I	0.46	0/1744	0.62	0/2364
1	J	0.47	0/1747	0.64	0/2369
1	K	0.54	0/1721	0.70	0/2335
1	L	0.59	0/1764	0.74	0/2392
All	All	0.49	0/21007	0.64	0/28481

There are no bond length outliers.

There are no bond angle outliers.

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	1718	0	1658	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1706	0	1652	9	0
1	C	1710	0	1651	16	0
1	D	1718	0	1658	2	0
1	E	1700	0	1644	5	0
1	F	1722	0	1664	9	0
1	G	1701	0	1651	6	0
1	H	1716	0	1661	11	0
1	I	1703	0	1648	10	0
1	J	1700	0	1646	5	0
1	K	1680	0	1613	20	0
1	L	1722	0	1664	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	3	0	0	0	0
2	J	1	0	0	0	0
2	L	2	0	0	0	0
3	A	10	0	16	3	0
3	C	10	0	15	1	0
3	F	10	0	15	2	0
3	G	10	0	15	2	0
3	I	10	0	15	2	0
3	L	10	0	15	4	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	F	5	0	0	0	0
5	C	6	0	8	3	0
5	I	6	0	8	1	0
5	L	6	0	8	1	0
6	A	108	0	0	1	0
6	B	73	0	0	0	0
6	C	117	0	0	0	0
6	D	93	0	0	0	0
6	E	79	0	0	1	0
6	F	79	0	0	0	0
6	G	93	0	0	0	0
6	H	69	0	0	1	0
6	I	66	0	0	1	0
6	J	83	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	58	0	0	0	0
6	L	67	0	0	2	0
All	All	21588	0	19925	120	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 3.

The worst 5 of 120 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:K:110:LEU:HD21	1:K:194:VAL:HG11	1.45	0.97
1:L:62:CYS:H	1:L:138:GLN:HE22	1.15	0.93
1:F:132:ASN:HD22	1:F:170:GLN:HE21	1.19	0.87
1:K:101:GLU:HB3	1:K:105:LEU:HB2	1.54	0.86
1:C:39:TYR:OH	5:C:1221:GOL:H2	1.81	0.80

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	208/215 (97%)	203 (98%)	5 (2%)	0	100	100
1	B	206/215 (96%)	201 (98%)	4 (2%)	1 (0%)	32	26
1	C	202/215 (94%)	198 (98%)	3 (2%)	1 (0%)	32	26
1	D	208/215 (97%)	203 (98%)	4 (2%)	1 (0%)	32	26
1	E	205/215 (95%)	202 (98%)	3 (2%)	0	100	100
1	F	208/215 (97%)	204 (98%)	3 (1%)	1 (0%)	32	26
1	G	206/215 (96%)	199 (97%)	6 (3%)	1 (0%)	32	26
1	H	208/215 (97%)	202 (97%)	5 (2%)	1 (0%)	32	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	206/215 (96%)	199 (97%)	7 (3%)	0	100	100
1	J	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	32	26
1	K	204/215 (95%)	189 (93%)	13 (6%)	2 (1%)	18	10
1	L	208/215 (97%)	195 (94%)	12 (6%)	1 (0%)	32	26
All	All	2476/2580 (96%)	2396 (97%)	70 (3%)	10 (0%)	38	33

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	53	ASP
1	K	64	ASN
1	B	64	ASN
1	D	64	ASN
1	F	64	ASN

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	194/197 (98%)	194 (100%)	0	100	100
1	B	192/197 (98%)	188 (98%)	4 (2%)	59	62
1	C	192/197 (98%)	184 (96%)	8 (4%)	34	30
1	D	194/197 (98%)	191 (98%)	3 (2%)	70	74
1	E	191/197 (97%)	187 (98%)	4 (2%)	59	62
1	F	194/197 (98%)	192 (99%)	2 (1%)	80	84
1	G	192/197 (98%)	187 (97%)	5 (3%)	51	52
1	H	194/197 (98%)	189 (97%)	5 (3%)	51	52
1	I	192/197 (98%)	189 (98%)	3 (2%)	68	72
1	J	192/197 (98%)	188 (98%)	4 (2%)	59	62
1	K	188/197 (95%)	182 (97%)	6 (3%)	44	42
1	L	194/197 (98%)	186 (96%)	8 (4%)	35	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2309/2364 (98%)	2257 (98%)	52 (2%)	59 58

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	172	GLN
1	H	159	GLN
1	L	153	THR
1	G	209[A]	THR
1	H	38	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	18	GLN
1	G	204	GLN
1	L	170	GLN
1	F	104	GLN
1	F	170	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SPD	A	1223	1	9,9,9	0.71	0	8,8,8	0.76	0
4	PO4	B	1220	-	4,4,4	2.14	1 (25%)	6,6,6	0.35	0
5	GOL	C	1221	-	5,5,5	0.22	0	5,5,5	0.39	0
4	PO4	C	1222	-	4,4,4	1.86	1 (25%)	6,6,6	0.52	0
3	SPD	C	1223	1	9,9,9	0.63	0	8,8,8	1.01	1 (12%)
4	PO4	F	1222	-	4,4,4	2.13	1 (25%)	6,6,6	0.36	0
3	SPD	F	1223	1	9,9,9	0.72	0	8,8,8	1.17	1 (12%)
3	SPD	G	1220	1	9,9,9	0.89	0	8,8,8	0.62	0
5	GOL	I	1220	-	5,5,5	0.17	0	5,5,5	0.47	0
3	SPD	I	1221	1	9,9,9	0.67	0	8,8,8	0.72	0
5	GOL	L	1222	-	5,5,5	0.13	0	5,5,5	0.38	0
3	SPD	L	1223	1	9,9,9	0.70	0	8,8,8	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SPD	A	1223	1	-	0/7/7/7	0/0/0/0
4	PO4	B	1220	-	-	0/0/0/0	0/0/0/0
5	GOL	C	1221	-	-	0/4/4/4	0/0/0/0
4	PO4	C	1222	-	-	0/0/0/0	0/0/0/0
3	SPD	C	1223	1	-	0/7/7/7	0/0/0/0
4	PO4	F	1222	-	-	0/0/0/0	0/0/0/0
3	SPD	F	1223	1	-	0/7/7/7	0/0/0/0
3	SPD	G	1220	1	-	0/7/7/7	0/0/0/0
5	GOL	I	1220	-	-	0/4/4/4	0/0/0/0
3	SPD	I	1221	1	-	0/7/7/7	0/0/0/0
5	GOL	L	1222	-	-	0/4/4/4	0/0/0/0
3	SPD	L	1223	1	-	0/7/7/7	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1222	PO4	P-O1	2.32	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1222	PO4	P-O1	3.02	1.57	1.50
4	B	1220	PO4	P-O1	3.03	1.57	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1223	SPD	C8-C7-N6	-3.11	104.12	112.06
3	C	1223	SPD	C8-C7-N6	-2.58	105.49	112.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1223	SPD	3	0
5	C	1221	GOL	3	0
3	C	1223	SPD	1	0
3	F	1223	SPD	2	0
3	G	1220	SPD	2	0
5	I	1220	GOL	1	0
3	I	1221	SPD	2	0
5	L	1222	GOL	1	0
3	L	1223	SPD	4	0

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	208/215 (96%)	0.03	2 (0%) 82 82	22, 37, 65, 88	0
1	B	208/215 (96%)	0.33	8 (3%) 41 41	21, 47, 87, 100	0
1	C	205/215 (95%)	0.01	2 (0%) 82 82	20, 37, 67, 88	0
1	D	208/215 (96%)	0.16	2 (0%) 82 82	23, 45, 76, 102	0
1	E	206/215 (95%)	0.25	3 (1%) 74 73	24, 46, 75, 83	0
1	F	209/215 (97%)	0.19	4 (1%) 67 66	27, 49, 81, 116	0
1	G	207/215 (96%)	0.15	5 (2%) 59 59	24, 43, 71, 87	0
1	H	208/215 (96%)	0.21	6 (2%) 52 52	24, 43, 77, 98	0
1	I	207/215 (96%)	0.63	19 (9%) 10 10	28, 58, 104, 121	0
1	J	207/215 (96%)	0.19	5 (2%) 59 59	22, 43, 76, 93	0
1	K	206/215 (95%)	1.70	64 (31%) 0 1	38, 62, 91, 112	0
1	L	209/215 (97%)	1.53	54 (25%) 1 1	31, 55, 87, 104	0
All	All	2488/2580 (96%)	0.45	174 (6%) 17 17	20, 47, 84, 121	0

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	187	VAL	12.7
1	K	187	VAL	9.1
1	K	105	LEU	9.0
1	K	100	ILE	7.4
1	L	150	ILE	7.2

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CL	B	1221	1/1	0.80	0.26	6.11	78,78,78,78	0
3	SPD	A	1223	10/10	0.97	0.16	3.69	22,25,28,33	0
4	PO4	F	1222	5/5	0.83	0.20	3.41	80,80,81,82	0
4	PO4	B	1220	5/5	0.84	0.26	3.35	86,88,90,90	0
5	GOL	I	1220	6/6	0.85	0.19	3.31	59,71,73,74	0
3	SPD	G	1220	10/10	0.97	0.16	2.19	29,32,33,33	0
3	SPD	F	1223	10/10	0.95	0.15	1.61	23,30,34,36	0
3	SPD	C	1223	10/10	0.96	0.14	1.61	23,28,31,33	0
3	SPD	I	1221	10/10	0.97	0.14	1.05	24,28,36,40	0
3	SPD	L	1223	10/10	0.84	0.25	0.99	40,45,48,51	0
4	PO4	C	1222	5/5	0.97	0.13	0.73	52,54,57,58	0
2	CL	A	1222	1/1	0.92	0.16	0.61	72,72,72,72	0
5	GOL	C	1221	6/6	0.85	0.17	0.36	36,51,55,56	0
2	CL	H	1223	1/1	0.78	0.13	0.19	79,79,79,79	0
2	CL	J	1220	1/1	0.99	0.14	0.05	31,31,31,31	0
2	CL	F	1221	1/1	0.98	0.12	-1.13	37,37,37,37	0
2	CL	C	1220	1/1	1.00	0.10	-1.51	29,29,29,29	0
2	CL	H	1221	1/1	0.99	0.10	-1.86	33,33,33,33	0
2	CL	A	1221	1/1	1.00	0.10	-2.37	27,27,27,27	0
2	CL	L	1221	1/1	0.97	0.11	-2.62	40,40,40,40	0
2	CL	G	1221	1/1	0.97	0.21	-	56,56,56,56	0
5	GOL	L	1222	6/6	0.62	0.17	-	66,69,72,72	0
2	CL	E	1220	1/1	0.95	0.18	-	69,69,69,69	0
2	CL	B	1222	1/1	0.96	0.23	-	58,58,58,58	0
2	CL	H	1222	1/1	0.90	0.12	-	82,82,82,82	0
2	CL	L	1224	1/1	0.94	0.07	-	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.