



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:01 AM UTC

PDB ID : 4C0Z / pdb_00004c0z
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 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:

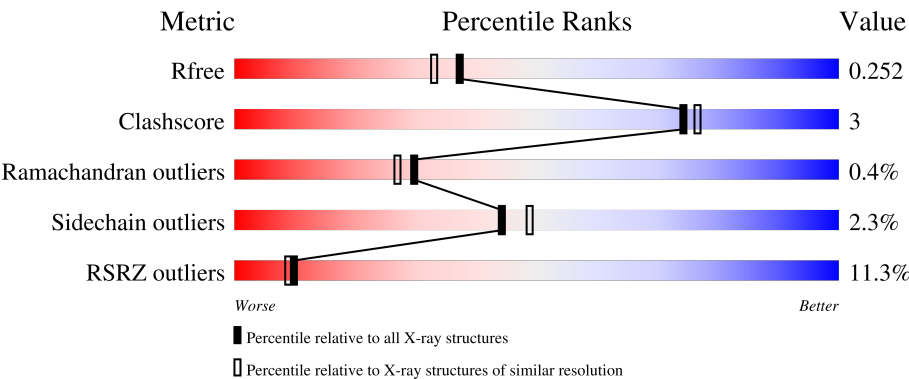
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	215	3% 93% • •
1	B	215	7% 89% 7% • •
1	C	215	3% 81% 13% • 5%
1	D	215	4% 92% 5% •
1	E	215	5% 91% 5% •

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Mol	Chain	Length	Quality of chain
1	F	215	
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
4	PO4	B	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 (CCD ID: CL) (formula: Cl).

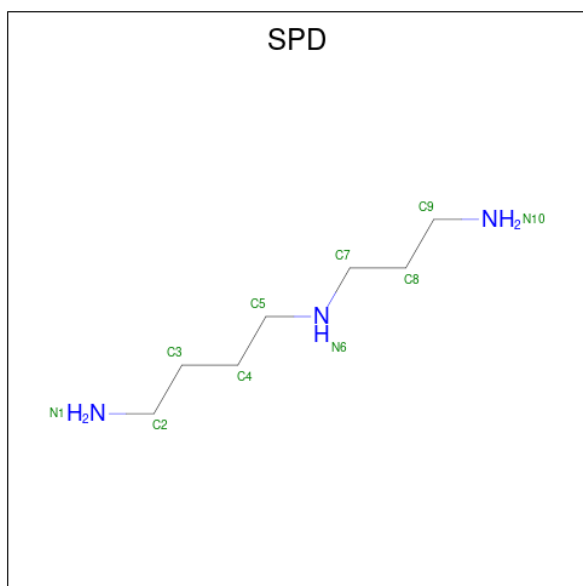
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	2	Total	Cl	0	0
			2	2		

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

- Molecule 3 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



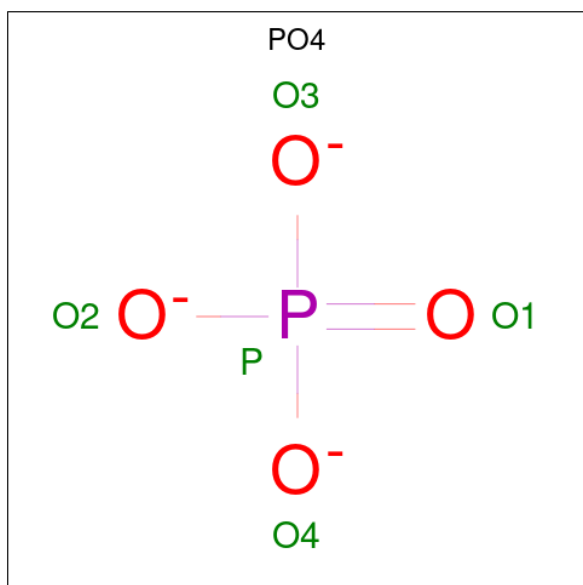
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	7	3		
3	C	1	Total	C	N	0	0
			10	7	3		
3	F	1	Total	C	N	0	0
			10	7	3		
3	G	1	Total	C	N	0	0
			10	7	3		

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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 (CCD ID: PO4) (formula: O_4P).



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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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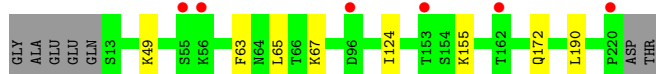
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	83	Total 83	O 83	0	0
6	K	58	Total 58	O 58	0	0
6	L	67	Total 67	O 67	0	0

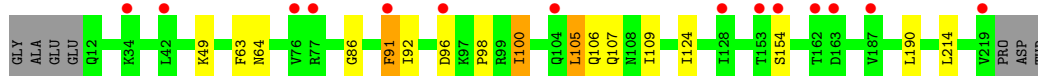
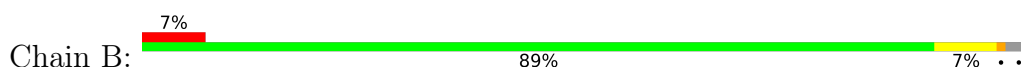
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

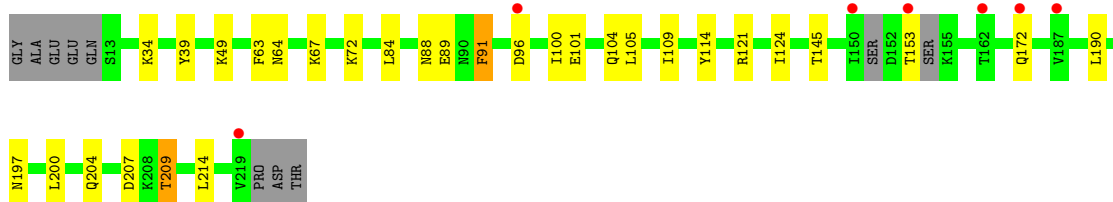
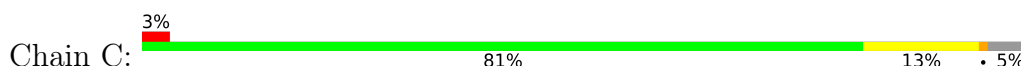
• Molecule 1: ANCILLARY PROTEIN 2



• Molecule 1: ANCILLARY PROTEIN 2



• Molecule 1: ANCILLARY PROTEIN 2

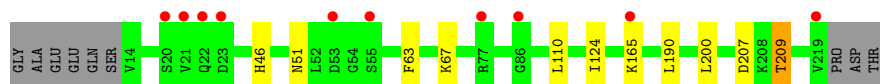


• Molecule 1: ANCILLARY PROTEIN 2

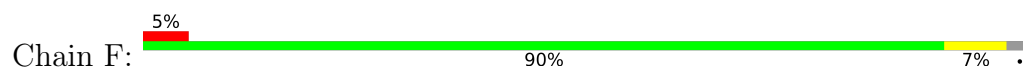


• Molecule 1: ANCILLARY PROTEIN 2

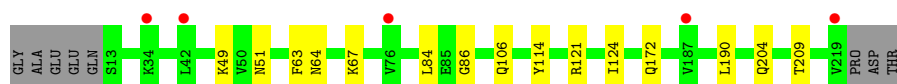
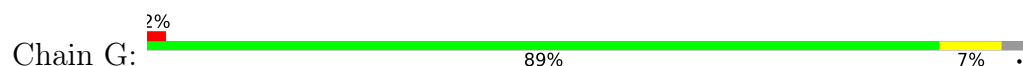




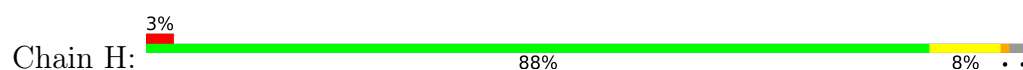
• Molecule 1: ANCILLARY PROTEIN 2



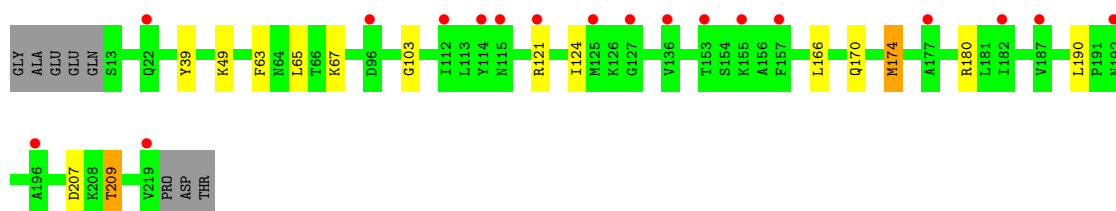
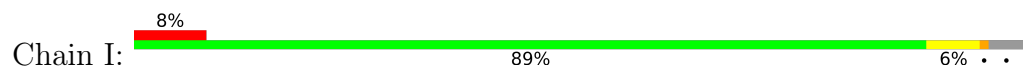
• Molecule 1: ANCILLARY PROTEIN 2



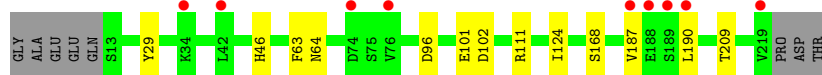
• Molecule 1: ANCILLARY PROTEIN 2



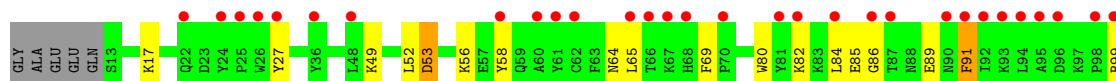
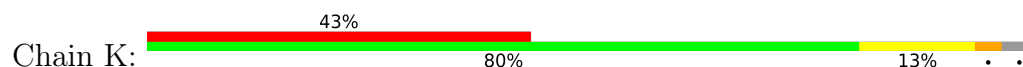
• Molecule 1: ANCILLARY PROTEIN 2

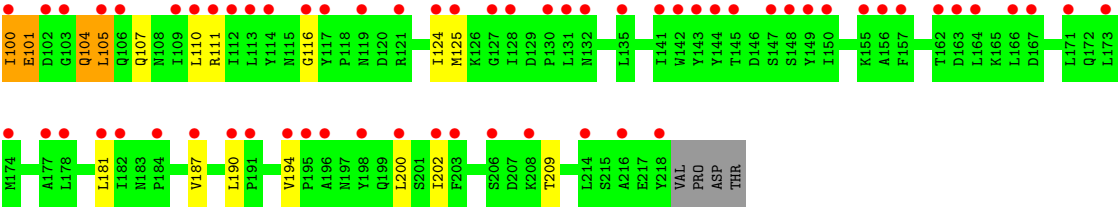


• Molecule 1: ANCILLARY PROTEIN 2

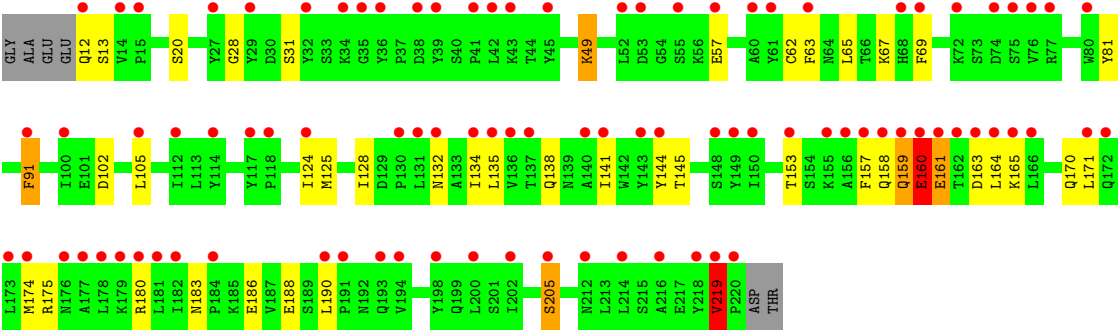
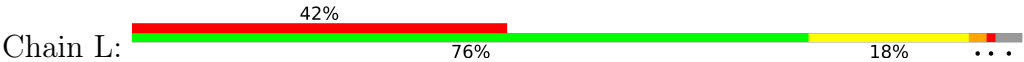


• Molecule 1: ANCILLARY PROTEIN 2





● 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) 99.9 (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	9253 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.6	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, 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	0.80	0/1760	1.11	1/2387 (0.0%)
1	B	0.79	0/1747	1.17	4/2368 (0.2%)
1	C	0.82	0/1753	1.15	2/2373 (0.1%)
1	D	0.78	0/1760	1.12	2/2387 (0.1%)
1	E	0.79	0/1741	1.16	2/2360 (0.1%)
1	F	0.80	0/1764	1.14	1/2392 (0.0%)
1	G	0.77	0/1745	1.12	2/2366 (0.1%)
1	H	0.78	0/1761	1.14	4/2388 (0.2%)
1	I	0.78	1/1744 (0.1%)	1.15	1/2364 (0.0%)
1	J	0.78	0/1747	1.14	2/2369 (0.1%)
1	K	0.91	0/1721	1.30	4/2335 (0.2%)
1	L	0.98	3/1764 (0.2%)	1.32	11/2392 (0.5%)
All	All	0.82	4/21007 (0.0%)	1.17	36/28481 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	219	VAL	CA-C	8.70	1.62	1.52
1	I	174	MET	SD-CE	-5.35	1.66	1.79
1	L	160	GLU	CA-C	5.35	1.59	1.52
1	L	205	SER	CA-C	5.01	1.59	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	209	THR	N-CA-C	-7.22	104.07	113.17
1	L	91	PHE	CA-CB-CG	-7.16	106.64	113.80
1	L	102	ASP	CA-CB-CG	7.12	119.72	112.60
1	E	63	PHE	CA-CB-CG	6.94	120.74	113.80
1	J	63	PHE	CA-CB-CG	6.77	120.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	63	PHE	CA-CB-CG	6.72	120.52	113.80
1	C	96	ASP	CA-CB-CG	6.67	119.27	112.60
1	D	63	PHE	CA-CB-CG	6.57	120.37	113.80
1	H	96	ASP	CA-CB-CG	6.55	119.15	112.60
1	L	63	PHE	CA-CB-CG	6.50	120.30	113.80
1	D	96	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	63	PHE	CA-CB-CG	6.24	120.04	113.80
1	B	96	ASP	CA-CB-CG	6.19	118.79	112.60
1	F	63	PHE	CA-CB-CG	6.13	119.93	113.80
1	K	91	PHE	CA-C-N	5.97	128.95	120.53
1	K	91	PHE	C-N-CA	5.97	128.95	120.53
1	I	63	PHE	CA-CB-CG	5.96	119.76	113.80
1	B	105	LEU	CA-C-N	5.91	128.48	120.38
1	B	105	LEU	C-N-CA	5.91	128.48	120.38
1	B	63	PHE	CA-CB-CG	5.75	119.55	113.80
1	H	63	PHE	CA-CB-CG	5.75	119.55	113.80
1	C	63	PHE	CA-CB-CG	5.63	119.43	113.80
1	L	161	GLU	CA-C-N	5.35	131.33	121.70
1	L	161	GLU	C-N-CA	5.35	131.33	121.70
1	L	219	VAL	N-CA-C	5.35	120.43	108.88
1	L	134	ILE	CA-C-N	5.32	127.72	120.54
1	L	134	ILE	C-N-CA	5.32	127.72	120.54
1	H	176	ASN	CA-CB-CG	5.28	117.88	112.60
1	L	183	ASN	CA-CB-CG	5.27	117.87	112.60
1	J	96	ASP	CA-CB-CG	5.26	117.86	112.60
1	E	51	ASN	CA-CB-CG	5.21	117.81	112.60
1	H	51	ASN	CA-CB-CG	5.18	117.78	112.60
1	G	51	ASN	CA-CB-CG	5.16	117.76	112.60
1	L	160	GLU	CA-C-N	5.16	130.99	121.70
1	L	160	GLU	C-N-CA	5.16	130.99	121.70
1	K	104	GLN	CA-C-O	-5.04	116.14	121.78

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
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	11	0
1	J	1700	0	1646	5	0
1	K	1680	0	1613	23	0
1	L	1722	0	1664	30	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	16	1	0
3	F	10	0	15	2	0
3	G	10	0	15	2	0
3	I	10	0	16	2	0
3	L	10	0	16	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	19928	125	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.

All (125) 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:K:125:MET:HE1	1:K:181:LEU:HD11	1.61	0.82
1:C:39:TYR:OH	5:C:1221:GOL:H2	1.81	0.80
1:C:91[A]:PHE:HE2	1:C:200:LEU:HD21	1.48	0.79
1:K:110:LEU:CD2	1:K:194:VAL:HG11	2.15	0.76
1:J:111:ARG:HD3	6:J:2056:HOH:O	1.87	0.72
1:B:154:SER:CB	1:I:103:GLY:HA3	2.20	0.70
1:L:160:GLU:N	1:L:161:GLU:HA	2.06	0.69
1:B:154:SER:HB2	1:I:103:GLY:HA3	1.73	0.69
1:H:108:ASN:HD22	1:H:111:ARG:HH12	1.41	0.69
1:H:108:ASN:HD22	1:H:111:ARG:NH1	1.90	0.69
1:K:99:ARG:HG2	1:K:100:ILE:H	1.59	0.66
1:F:129:ASP:H	1:F:170:GLN:HE22	1.44	0.66
1:C:89:GLU:HG3	1:F:185:LYS:HD3	1.78	0.63
1:B:91:PHE:HZ	1:B:214:LEU:HD11	1.64	0.62
1:L:62:CYS:N	1:L:138:GLN:HE22	1.92	0.61
1:C:88:ASN:HD21	1:C:104:GLN:HG3	1.66	0.61
1:H:104:GLN:HB2	1:H:107:GLN:HB2	1.83	0.60
1:L:57[A]:GLU:HG3	6:L:2022:HOH:O	2.00	0.60
1:C:91[B]:PHE:CZ	1:C:145:THR:HG22	2.36	0.60
1:G:86:GLY:O	1:G:106:GLN:HG3	2.02	0.60
1:I:65:LEU:O	3:I:1221:SPD:H51	2.02	0.60
1:C:91[A]:PHE:HZ	1:C:214:LEU:HD22	1.67	0.59
1:C:91[A]:PHE:CE2	1:C:200:LEU:HD21	2.36	0.59
1:K:107:GLN:O	1:K:111:ARG:HG2	2.02	0.58
1:L:67:LYS:O	3:L:1223:SPD:H52	2.04	0.58
1:L:219:VAL:HG12	1:L:219:VAL:O	2.03	0.58
1:E:207:ASP:OD1	1:E:209:THR:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:HE2	1:K:104:GLN:HG3	1.86	0.56
1:E:124:ILE:HD11	1:E:190:LEU:HD11	1.87	0.56
1:K:116:GLY:HA2	1:K:125:MET:HE3	1.88	0.56
1:L:160:GLU:H	1:L:161:GLU:HA	1.68	0.56
1:C:67:LYS:O	3:C:1223:SPD:H42	2.06	0.56
1:H:217:GLU:HB2	6:H:2068:HOH:O	2.05	0.55
1:B:154:SER:HB3	1:I:103:GLY:HA3	1.89	0.54
1:G:67:LYS:O	3:G:1220:SPD:H51	2.08	0.53
1:L:62:CYS:H	1:L:138:GLN:NE2	1.96	0.53
1:H:187:VAL:HG13	1:H:190:LEU:HD12	1.90	0.53
1:F:124:ILE:HD11	1:F:190:LEU:HD11	1.91	0.52
1:L:91:PHE:CZ	1:L:145:THR:HG22	2.44	0.52
1:G:67:LYS:O	3:G:1220:SPD:C5	2.58	0.52
1:C:34:LYS:HG3	5:C:1221:GOL:H31	1.90	0.52
1:I:124:ILE:HD11	1:I:190:LEU:HD11	1.92	0.52
1:L:124:ILE:HD11	1:L:190:LEU:HD21	1.92	0.52
1:C:124:ILE:HD11	1:C:190:LEU:HD11	1.92	0.51
1:F:169:GLN:HG3	1:I:180:ARG:HD2	1.92	0.51
1:K:27:TYR:HB2	1:K:80:TRP:CZ3	2.45	0.51
1:C:84:LEU:HD11	1:C:204:GLN:HE21	1.75	0.51
1:B:124:ILE:HD11	1:B:190:LEU:HD11	1.93	0.51
1:L:171:LEU:HD22	5:L:1222:GOL:H12	1.93	0.51
1:A:124:ILE:HD11	1:A:190:LEU:HD11	1.91	0.50
1:K:111:ARG:HB3	1:K:187:VAL:HG11	1.91	0.50
6:I:2036:HOH:O	1:J:46:HIS:HE1	1.93	0.49
1:L:67:LYS:O	3:L:1223:SPD:C5	2.60	0.49
1:D:124:ILE:HD11	1:D:190:LEU:HD11	1.94	0.49
1:D:207:ASP:OD1	1:D:209:THR:HB	2.12	0.49
1:L:132:ASN:HD22	1:L:170:GLN:NE2	2.10	0.49
1:I:67:LYS:O	3:I:1221:SPD:H52	2.13	0.49
1:C:91[A]:PHE:CZ	1:C:109:ILE:HD13	2.48	0.49
1:J:124:ILE:HD11	1:J:190:LEU:HD11	1.95	0.48
1:K:86:GLY:HA2	1:K:202:ILE:HG13	1.94	0.48
1:I:166:LEU:HD22	1:I:174:MET:HE1	1.96	0.48
1:L:132:ASN:HD22	1:L:170:GLN:HE21	1.61	0.48
1:L:135:LEU:HD13	1:L:174:MET:HE1	1.96	0.47
1:F:129:ASP:H	1:F:170:GLN:NE2	2.12	0.47
1:G:124:ILE:HD11	1:G:190:LEU:HD11	1.96	0.47
1:I:170:GLN:HB3	1:I:174:MET:HE2	1.95	0.47
1:A:172:GLN:HG2	6:A:2094:HOH:O	2.15	0.47
1:K:27:TYR:HB2	1:K:80:TRP:HZ3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:ILE:HD11	1:L:190:LEU:CD2	2.44	0.46
1:E:46:HIS:HE1	6:E:2018:HOH:O	1.96	0.46
1:C:72:LYS:HD2	5:C:1221:GOL:H12	1.98	0.46
1:H:124:ILE:HD11	1:H:190:LEU:HD11	1.97	0.46
1:K:82:LYS:HE3	1:K:84:LEU:HD21	1.98	0.45
1:B:98:PRO:HG2	1:B:100:ILE:HD12	1.98	0.45
1:E:67:LYS:O	3:F:1223:SPD:H71	2.17	0.45
1:L:171:LEU:HD21	1:L:175:ARG:CZ	2.47	0.45
1:K:125:MET:CE	1:K:181:LEU:HD11	2.37	0.45
1:L:28:GLY:HA3	1:L:81:TYR:CE1	2.52	0.45
1:F:207:ASP:OD1	1:F:209:THR:HB	2.17	0.45
1:K:99:ARG:HG2	1:K:100:ILE:HG13	1.99	0.45
1:L:69:PHE:CE2	3:L:1223:SPD:H41	2.52	0.45
1:H:187:VAL:HA	1:H:190:LEU:HD12	1.98	0.44
1:L:81:TYR:CE2	1:L:205:SER:HB2	2.52	0.44
1:L:157:PHE:HB2	6:L:2058:HOH:O	2.17	0.44
1:C:114:TYR:CZ	1:C:121:ARG:HG2	2.52	0.44
1:H:207:ASP:OD1	1:H:209:THR:HB	2.18	0.44
1:G:114:TYR:CZ	1:G:121:ARG:HG2	2.52	0.44
1:H:160:GLU:HB3	1:H:164:LEU:HD12	2.00	0.44
1:L:180:ARG:HG2	1:L:186:GLU:HG2	1.98	0.44
1:C:197:ASN:HB3	1:J:102:ASP:O	2.18	0.44
1:A:65:LEU:O	3:A:1223:SPD:H51	2.17	0.44
1:H:108:ASN:HA	1:H:111:ARG:NH1	2.32	0.44
1:J:29:TYR:CD1	1:J:29:TYR:N	2.86	0.44
1:L:105:LEU:CD1	1:L:144:TYR:HB3	2.48	0.43
1:F:67:LYS:O	3:F:1223:SPD:H42	2.18	0.43
1:C:207:ASP:OD1	1:C:209:THR:HB	2.18	0.43
1:L:49:LYS:HG2	1:L:57[A]:GLU:HB2	2.00	0.43
1:L:158:GLN:HB2	1:L:159:GLN:HA	2.00	0.43
1:G:84:LEU:HD11	1:G:204:GLN:HE21	1.83	0.43
1:I:207:ASP:OD1	1:I:209:THR:HB	2.19	0.43
1:L:125:MET:HA	1:L:128:ILE:HD12	2.01	0.43
1:K:124:ILE:HG22	1:K:125:MET:HE2	2.00	0.42
1:H:164:LEU:O	1:H:165:LYS:HG2	2.20	0.42
1:B:86:GLY:O	1:B:106:GLN:HG3	2.20	0.42
1:L:12:GLN:HB2	1:L:31:SER:HB2	2.01	0.42
1:B:92:ILE:HG12	1:B:100:ILE:HD11	2.01	0.42
1:E:110:LEU:HG	1:E:200:LEU:HB2	2.02	0.42
1:L:164:LEU:O	1:L:165:LYS:HG2	2.20	0.42
1:K:91:PHE:CZ	1:K:200:LEU:HD21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:LEU:HB3	1:L:65:LEU:HB3	2.02	0.41
1:F:82:LYS:O	1:F:84:LEU:HD22	2.20	0.41
1:K:56:LYS:HD3	1:K:58:TYR:CZ	2.56	0.41
1:I:39:TYR:OH	5:I:1220:GOL:H32	2.20	0.41
1:K:69:PHE:CE1	3:L:1223:SPD:H91	2.55	0.41
1:B:91:PHE:CZ	1:B:214:LEU:HD11	2.49	0.41
1:A:67:LYS:O	3:A:1223:SPD:H71	2.21	0.41
1:K:52:LEU:O	1:K:53:ASP:C	2.64	0.41
1:L:170:GLN:O	1:L:174:MET:HG3	2.22	0.40
1:A:67:LYS:O	3:A:1223:SPD:H52	2.21	0.40
1:K:17:LYS:HD2	1:K:27:TYR:CZ	2.56	0.40
1:K:124:ILE:HD11	1:K:190:LEU:HD11	2.02	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	208/215 (97%)	203 (98%)	5 (2%)	0	100	100
1	B	206/215 (96%)	201 (98%)	4 (2%)	1 (0%)	24	21
1	C	202/215 (94%)	198 (98%)	3 (2%)	1 (0%)	24	21
1	D	208/215 (97%)	203 (98%)	4 (2%)	1 (0%)	24	21
1	E	205/215 (95%)	202 (98%)	3 (2%)	0	100	100
1	F	208/215 (97%)	204 (98%)	3 (1%)	1 (0%)	24	21
1	G	206/215 (96%)	199 (97%)	6 (3%)	1 (0%)	24	21
1	H	208/215 (97%)	202 (97%)	5 (2%)	1 (0%)	24	21
1	I	206/215 (96%)	199 (97%)	7 (3%)	0	100	100
1	J	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	24	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	204/215 (95%)	189 (93%)	13 (6%)	2 (1%)	12	8
1	L	208/215 (97%)	195 (94%)	12 (6%)	1 (0%)	24	21
All	All	2476/2580 (96%)	2396 (97%)	70 (3%)	10 (0%)	30	27

All (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
1	G	64	ASN
1	H	64	ASN
1	J	64	ASN
1	C	64	ASN
1	L	219	VAL

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%)	193 (100%)	1 (0%)	81	87
1	B	192/197 (98%)	186 (97%)	6 (3%)	35	37
1	C	192/197 (98%)	182 (95%)	10 (5%)	21	18
1	D	194/197 (98%)	189 (97%)	5 (3%)	40	44
1	E	191/197 (97%)	189 (99%)	2 (1%)	68	75
1	F	194/197 (98%)	192 (99%)	2 (1%)	68	75
1	G	192/197 (98%)	188 (98%)	4 (2%)	47	52
1	H	194/197 (98%)	191 (98%)	3 (2%)	57	64
1	I	192/197 (98%)	189 (98%)	3 (2%)	55	62
1	J	192/197 (98%)	188 (98%)	4 (2%)	47	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	188/197 (95%)	182 (97%)	6 (3%)	34	35
1	L	194/197 (98%)	185 (95%)	9 (5%)	24	22
All	All	2309/2364 (98%)	2254 (98%)	55 (2%)	44	47

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	B	49	LYS
1	B	91	PHE
1	B	100	ILE
1	B	105	LEU
1	B	107	GLN
1	B	109	ILE
1	C	49	LYS
1	C	91[A]	PHE
1	C	91[B]	PHE
1	C	100	ILE
1	C	101	GLU
1	C	105	LEU
1	C	153	THR
1	C	172[A]	GLN
1	C	172[B]	GLN
1	C	209	THR
1	D	49	LYS
1	D	101	GLU
1	D	119	ASN
1	D	155	LYS
1	D	209	THR
1	E	165	LYS
1	E	209	THR
1	F	49	LYS
1	F	209	THR
1	G	49	LYS
1	G	172	GLN
1	G	209[A]	THR
1	G	209[B]	THR
1	H	96	ASP
1	H	101	GLU
1	H	209	THR
1	I	49	LYS

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Mol	Chain	Res	Type
1	I	121	ARG
1	I	209	THR
1	J	101	GLU
1	J	168	SER
1	J	187	VAL
1	J	209	THR
1	K	49	LYS
1	K	85	GLU
1	K	89	GLU
1	K	100	ILE
1	K	101	GLU
1	K	105	LEU
1	L	13	SER
1	L	20	SER
1	L	49	LYS
1	L	141	ILE
1	L	153	THR
1	L	159	GLN
1	L	160	GLU
1	L	163	ASP
1	L	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	B	18	GLN
1	B	119	ASN
1	B	172	GLN
1	C	46	HIS
1	C	88	ASN
1	C	104	GLN
1	C	106	GLN
1	C	183	ASN
1	C	204	GLN
1	D	18	GLN
1	D	104	GLN
1	D	172	GLN
1	E	46	HIS
1	E	172	GLN
1	E	204	GLN
1	F	12	GLN

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Mol	Chain	Res	Type
1	F	18	GLN
1	F	107	GLN
1	F	170	GLN
1	F	172	GLN
1	F	183	ASN
1	F	204	GLN
1	G	106	GLN
1	G	204	GLN
1	H	18	GLN
1	H	108	ASN
1	H	172	GLN
1	H	204	GLN
1	I	159	GLN
1	J	46	HIS
1	J	51	ASN
1	J	172	GLN
1	J	183	ASN
1	K	16	ASN
1	K	18	GLN
1	K	64	ASN
1	K	107	GLN
1	K	172	GLN
1	K	183	ASN
1	L	12	GLN
1	L	18	GLN
1	L	132	ASN
1	L	138	GLN
1	L	159	GLN
1	L	170	GLN
1	L	204	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 [i](#)

There are no oligosaccharides 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	I	1221	1	9,9,9	0.67	0	8,8,8	0.75	0
3	SPD	C	1223	1	9,9,9	0.62	0	8,8,8	0.94	1 (12%)
5	GOL	L	1222	-	5,5,5	0.11	0	5,5,5	0.35	0
3	SPD	G	1220	1	9,9,9	0.88	0	8,8,8	0.59	0
4	PO4	B	1220	-	4,4,4	2.23	4 (100%)	6,6,6	0.41	0
3	SPD	L	1223	1	9,9,9	0.70	0	8,8,8	0.68	0
3	SPD	A	1223	1	9,9,9	0.70	0	8,8,8	0.73	0
5	GOL	I	1220	-	5,5,5	0.12	0	5,5,5	0.52	0
4	PO4	F	1222	-	4,4,4	2.22	2 (50%)	6,6,6	0.43	0
3	SPD	F	1223	1	9,9,9	0.72	0	8,8,8	1.11	1 (12%)
4	PO4	C	1222	-	4,4,4	1.98	1 (25%)	6,6,6	0.62	0
5	GOL	C	1221	-	5,5,5	0.20	0	5,5,5	0.37	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	I	1221	1	-	3/7/7/7	-
3	SPD	C	1223	1	-	2/7/7/7	-
5	GOL	L	1222	-	-	0/4/4/4	-
3	SPD	G	1220	1	-	4/7/7/7	-
3	SPD	L	1223	1	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SPD	A	1223	1	-	2/7/7/7	-
5	GOL	I	1220	-	-	0/4/4/4	-
3	SPD	F	1223	1	-	0/7/7/7	-
5	GOL	C	1221	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1220	PO4	P-O1	2.74	1.57	1.50
4	F	1222	PO4	P-O1	2.73	1.57	1.50
4	F	1222	PO4	P-O2	2.09	1.60	1.54
4	C	1222	PO4	P-O1	2.06	1.55	1.50
4	B	1220	PO4	P-O3	2.03	1.60	1.54
4	B	1220	PO4	P-O2	2.03	1.60	1.54
4	B	1220	PO4	P-O4	2.02	1.60	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1223	SPD	C8-C7-N6	-2.96	104.12	112.07
3	C	1223	SPD	C8-C7-N6	-2.45	105.49	112.07

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1221	SPD	C3-C4-C5-N6
3	A	1223	SPD	C3-C4-C5-N6
3	G	1220	SPD	N6-C7-C8-C9
3	L	1223	SPD	N6-C7-C8-C9
3	L	1223	SPD	C8-C7-N6-C5
3	I	1221	SPD	N1-C2-C3-C4
3	L	1223	SPD	C2-C3-C4-C5
3	G	1220	SPD	C2-C3-C4-C5
3	A	1223	SPD	C8-C7-N6-C5
3	G	1220	SPD	C8-C7-N6-C5
3	G	1220	SPD	C3-C4-C5-N6
3	C	1223	SPD	C3-C4-C5-N6
3	I	1221	SPD	C8-C7-N6-C5
3	C	1223	SPD	C8-C7-N6-C5

There are no ring outliers.

9 monomers are involved in 19 short contacts:

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

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	208/215 (96%)	0.10	6 (2%) 53 52	14, 37, 65, 88	2 (0%)
1	B	208/215 (96%)	0.47	14 (6%) 24 22	21, 47, 87, 100	0
1	C	205/215 (95%)	0.14	7 (3%) 48 47	20, 36, 67, 88	3 (1%)
1	D	208/215 (96%)	0.39	9 (4%) 40 39	23, 44, 76, 102	2 (0%)
1	E	206/215 (95%)	0.58	10 (4%) 35 34	24, 46, 75, 83	1 (0%)
1	F	209/215 (97%)	0.57	11 (5%) 32 31	27, 48, 81, 116	1 (0%)
1	G	207/215 (96%)	0.26	5 (2%) 59 59	20, 43, 71, 87	1 (0%)
1	H	208/215 (96%)	0.41	7 (3%) 48 47	24, 43, 76, 98	2 (0%)
1	I	207/215 (96%)	0.86	18 (8%) 16 15	19, 58, 104, 121	1 (0%)
1	J	207/215 (96%)	0.39	9 (4%) 40 39	22, 43, 76, 93	2 (0%)
1	K	206/215 (95%)	2.06	93 (45%) 0 1	38, 62, 91, 112	0
1	L	209/215 (97%)	1.98	91 (43%) 0 1	29, 55, 87, 104	1 (0%)
All	All	2488/2580 (96%)	0.69	280 (11%) 10 9	14, 47, 84, 121	16 (0%)

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	100	ILE	7.9
1	J	187	VAL	6.9
1	E	219	VAL	6.6
1	L	177	ALA	6.5
1	L	181	LEU	6.4
1	K	105	LEU	6.3
1	L	162	THR	5.7
1	L	157	PHE	5.5
1	K	198	TYR	5.2
1	C	219	VAL	4.9
1	L	153	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	L	150	ILE	4.7
1	K	144	TYR	4.7
1	L	164	LEU	4.6
1	G	219	VAL	4.5
1	K	142	TRP	4.3
1	L	124	ILE	4.3
1	L	149	TYR	4.3
1	B	219	VAL	4.2
1	K	106	GLN	4.2
1	H	187	VAL	4.2
1	L	14	VAL	4.2
1	K	66	THR	4.2
1	K	194	VAL	4.1
1	L	140	ALA	4.0
1	K	91	PHE	4.0
1	K	95	ALA	4.0
1	F	76	VAL	4.0
1	K	67	LYS	3.9
1	D	196	ALA	3.9
1	L	200	LEU	3.9
1	K	218	TYR	3.8
1	C	153	THR	3.7
1	E	22	GLN	3.7
1	L	156	ALA	3.7
1	K	195	PRO	3.7
1	K	182	ILE	3.7
1	K	90	ASN	3.7
1	I	187	VAL	3.7
1	J	219	VAL	3.7
1	K	84	LEU	3.6
1	L	131	LEU	3.6
1	K	109	ILE	3.6
1	L	194	VAL	3.5
1	L	32	TYR	3.5
1	K	200	LEU	3.4
1	L	105	LEU	3.4
1	L	45	TYR	3.4
1	L	112	ILE	3.4
1	K	114	TYR	3.4
1	L	76	VAL	3.4
1	F	20	SER	3.4
1	K	65	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	191	PRO	3.4
1	K	150	ILE	3.4
1	E	20	SER	3.3
1	I	219	VAL	3.3
1	L	12	GLN	3.3
1	H	91	PHE	3.3
1	C	162	THR	3.3
1	K	92	ILE	3.3
1	K	196	ALA	3.3
1	K	202	ILE	3.3
1	L	42	LEU	3.3
1	K	187	VAL	3.3
1	L	218	TYR	3.3
1	L	52	LEU	3.3
1	K	24	TYR	3.2
1	J	190	LEU	3.2
1	G	34	LYS	3.2
1	J	189	SER	3.2
1	L	57[A]	GLU	3.2
1	B	76	VAL	3.2
1	K	124	ILE	3.2
1	L	163	ASP	3.2
1	K	131	LEU	3.2
1	A	220	PRO	3.2
1	L	219	VAL	3.1
1	L	171	LEU	3.1
1	L	41	PRO	3.1
1	K	121	ARG	3.1
1	L	173	LEU	3.1
1	K	174	MET	3.1
1	L	161	GLU	3.1
1	K	110	LEU	3.1
1	K	164	LEU	3.1
1	K	181	LEU	3.0
1	K	190	LEU	3.0
1	L	137	THR	3.0
1	K	157	PHE	3.0
1	L	69	PHE	3.0
1	K	25	PRO	3.0
1	L	220	PRO	3.0
1	B	42	LEU	2.9
1	L	178	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	179	LYS	2.9
1	F	220	PRO	2.9
1	K	203	PHE	2.9
1	B	187	VAL	2.9
1	H	96	ASP	2.9
1	K	98	PRO	2.9
1	B	154	SER	2.9
1	K	61	TYR	2.9
1	K	117	TYR	2.9
1	K	116	GLY	2.9
1	J	42	LEU	2.8
1	K	208	LYS	2.8
1	L	72	LYS	2.8
1	K	149	TYR	2.8
1	K	171	LEU	2.8
1	K	173	LEU	2.8
1	A	162	THR	2.8
1	K	162	THR	2.8
1	B	96	ASP	2.8
1	K	166	LEU	2.8
1	B	162	THR	2.8
1	L	74	ASP	2.8
1	H	103	GLY	2.8
1	L	60	ALA	2.8
1	K	178	LEU	2.8
1	L	15	PRO	2.8
1	I	192	ASN	2.7
1	K	58	TYR	2.7
1	L	117	TYR	2.7
1	G	76	VAL	2.7
1	F	34	LYS	2.7
1	K	113	LEU	2.7
1	K	125	MET	2.7
1	B	34	LYS	2.7
1	I	127	GLY	2.7
1	L	172	GLN	2.7
1	L	193	GLN	2.7
1	K	102	ASP	2.7
1	K	163	ASP	2.7
1	L	182	ILE	2.7
1	L	135	LEU	2.6
1	J	74	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	148	SER	2.6
1	L	34	LYS	2.6
1	K	86	GLY	2.6
1	K	26	TRP	2.6
1	I	125	MET	2.6
1	D	190	LEU	2.6
1	L	39	TYR	2.6
1	L	180	ARG	2.6
1	K	141	ILE	2.6
1	K	48	LEU	2.6
1	L	190	LEU	2.6
1	K	111	ARG	2.6
1	I	112	ILE	2.6
1	K	81	TYR	2.6
1	K	96	ASP	2.6
1	L	118	PRO	2.6
1	K	135	LEU	2.6
1	L	63	PHE	2.5
1	E	21	VAL	2.5
1	G	187	VAL	2.5
1	L	141	ILE	2.5
1	I	196	ALA	2.5
1	L	174	MET	2.5
1	J	76	VAL	2.5
1	K	87	THR	2.5
1	I	136	VAL	2.5
1	K	177	ALA	2.5
1	H	190	LEU	2.5
1	B	91	PHE	2.5
1	L	91	PHE	2.5
1	L	80	TRP	2.5
1	C	172[A]	GLN	2.4
1	F	75	SER	2.4
1	K	93	LYS	2.4
1	C	150	ILE	2.4
1	L	158	GLN	2.4
1	K	147	SER	2.4
1	L	198	TYR	2.4
1	K	184	PRO	2.4
1	L	77	ARG	2.4
1	L	159	GLN	2.4
1	L	136	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	72	LYS	2.4
1	K	156	ALA	2.4
1	K	128	ILE	2.4
1	I	121	ARG	2.4
1	K	145	THR	2.4
1	K	143	TYR	2.3
1	L	61	TYR	2.3
1	L	144	TYR	2.3
1	K	119	ASN	2.3
1	K	132	ASN	2.3
1	L	35	GLY	2.3
1	E	53	ASP	2.3
1	I	157	PHE	2.3
1	J	34	LYS	2.3
1	H	92	ILE	2.3
1	F	187	VAL	2.3
1	L	205	SER	2.3
1	L	29	TYR	2.3
1	E	55	SER	2.3
1	L	68	HIS	2.3
1	D	76	VAL	2.3
1	D	219	VAL	2.3
1	K	27	TYR	2.3
1	E	77	ARG	2.3
1	E	86	GLY	2.3
1	G	42	LEU	2.3
1	K	155	LYS	2.3
1	L	165	LYS	2.3
1	L	134	ILE	2.3
1	B	163	ASP	2.3
1	K	60	ALA	2.3
1	K	216	ALA	2.3
1	K	94	LEU	2.3
1	K	214	LEU	2.3
1	L	214	LEU	2.3
1	L	75	SER	2.2
1	K	112	ILE	2.2
1	F	77	ARG	2.2
1	F	163	ASP	2.2
1	K	103	GLY	2.2
1	L	166	LEU	2.2
1	J	188	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	160	GLU	2.2
1	K	68	HIS	2.2
1	I	22	GLN	2.2
1	K	148	SER	2.2
1	I	182	ILE	2.2
1	L	176	ASN	2.2
1	C	187	VAL	2.2
1	C	96	ASP	2.2
1	K	127	GLY	2.2
1	K	22	GLN	2.2
1	I	114	TYR	2.2
1	I	155	LYS	2.2
1	K	82	LYS	2.2
1	L	212	ASN	2.2
1	F	74	ASP	2.2
1	B	77	ARG	2.2
1	L	55	SER	2.2
1	L	36	TYR	2.2
1	L	143	TYR	2.2
1	L	155	LYS	2.2
1	E	23	ASP	2.2
1	I	96	ASP	2.2
1	A	55	SER	2.1
1	K	167	ASP	2.1
1	L	53	ASP	2.1
1	B	104	GLN	2.1
1	D	105	LEU	2.1
1	E	165	LYS	2.1
1	L	43	LYS	2.1
1	K	70	PRO	2.1
1	L	130	PRO	2.1
1	B	128	ILE	2.1
1	F	42	LEU	2.1
1	K	206	SER	2.1
1	I	115	ASN	2.1
1	L	132	ASN	2.1
1	L	38	ASP	2.1
1	A	153	THR	2.1
1	B	153	THR	2.1
1	D	218	TYR	2.1
1	I	153	THR	2.1
1	K	36	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	114	TYR	2.1
1	L	191	PRO	2.1
1	L	202	ILE	2.1
1	I	177	ALA	2.1
1	K	62	CYS	2.0
1	K	99	ARG	2.0
1	D	220	PRO	2.0
1	K	130	PRO	2.0
1	A	56	LYS	2.0
1	L	27	TYR	2.0
1	L	100	ILE	2.0
1	D	154	SER	2.0
1	L	216	ALA	2.0
1	D	119	ASN	2.0
1	A	96	ASP	2.0
1	H	162	THR	2.0
1	L	184	PRO	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](#)

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	B	1220	5/5	0.65	0.15	86,88,90,90	0
5	GOL	L	1222	6/6	0.72	0.14	66,69,72,72	0
4	PO4	F	1222	5/5	0.76	0.12	80,80,81,82	0
5	GOL	I	1220	6/6	0.79	0.14	59,71,73,74	0
3	SPD	L	1223	10/10	0.79	0.18	40,45,48,51	0
2	CL	H	1222	1/1	0.83	0.13	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	L	1224	1/1	0.84	0.13	79,79,79,79	0
2	CL	H	1223	1/1	0.86	0.12	79,79,79,79	0
2	CL	A	1222	1/1	0.87	0.18	72,72,72,72	0
5	GOL	C	1221	6/6	0.89	0.11	36,51,55,56	0
2	CL	B	1221	1/1	0.91	0.19	78,78,78,78	0
4	PO4	C	1222	5/5	0.91	0.09	52,54,57,58	0
3	SPD	F	1223	10/10	0.93	0.09	23,30,34,36	0
3	SPD	I	1221	10/10	0.95	0.08	24,28,36,40	0
3	SPD	C	1223	10/10	0.95	0.08	23,28,31,33	0
2	CL	G	1221	1/1	0.95	0.18	56,56,56,56	0
3	SPD	G	1220	10/10	0.95	0.09	29,32,33,33	0
2	CL	F	1221	1/1	0.96	0.07	37,37,37,37	0
2	CL	B	1222	1/1	0.96	0.21	58,58,58,58	0
2	CL	L	1221	1/1	0.96	0.06	40,40,40,40	0
3	SPD	A	1223	10/10	0.97	0.06	22,25,28,33	0
2	CL	E	1220	1/1	0.97	0.23	69,69,69,69	0
2	CL	H	1221	1/1	0.99	0.05	33,33,33,33	0
2	CL	J	1220	1/1	0.99	0.04	31,31,31,31	0
2	CL	C	1220	1/1	1.00	0.03	29,29,29,29	0
2	CL	A	1221	1/1	1.00	0.03	27,27,27,27	0

6.5 Other polymers

There are no such residues in this entry.