Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 09:34 AM EDT

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 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 (i) 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 (i)) were used in the production of this report:

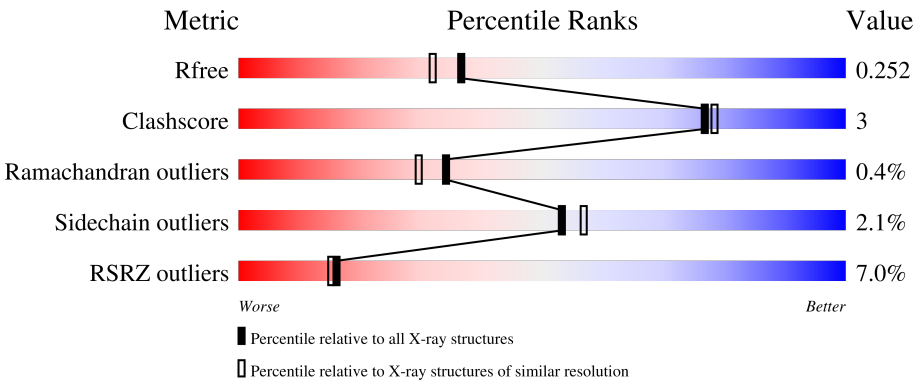
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	% 94% • •
1	B	215	4% 91% 5% • •
1	C	215	% 83% 11% • 5%
1	D	215	% 93% • •
1	E	215	% 91% 5% •

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Mol	Chain	Length	Quality of chain
1	F	215	2% 91% 6%
1	G	215	2% 90% 6%
1	H	215	2% 88% 8%
1	I	215	9% 90% 6%
1	J	215	2% 91% 5%
1	K	215	30% 80% 14%
1	L	215	25% 79% 17%

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 (i)

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

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

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

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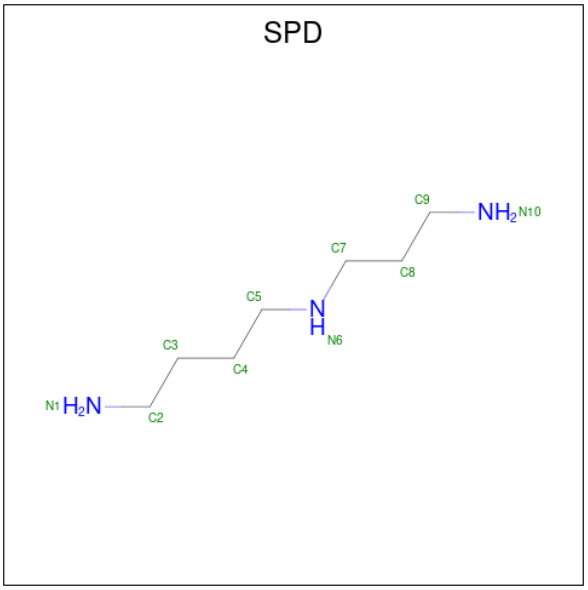
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	3	Total Cl 3 3	0	0
2	J	1	Total Cl 1 1	0	0
2	L	2	Total Cl 2 2	0	0

- 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 10 7 3	0	0
3	C	1	Total C N 10 7 3	0	0
3	F	1	Total C N 10 7 3	0	0
3	G	1	Total C N 10 7 3	0	0

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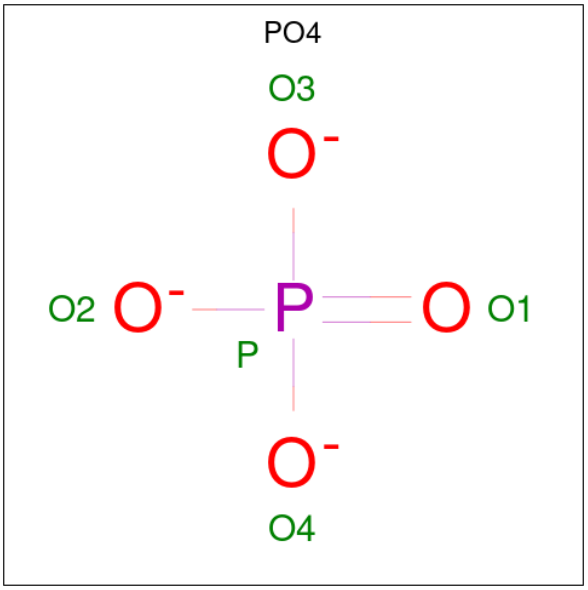
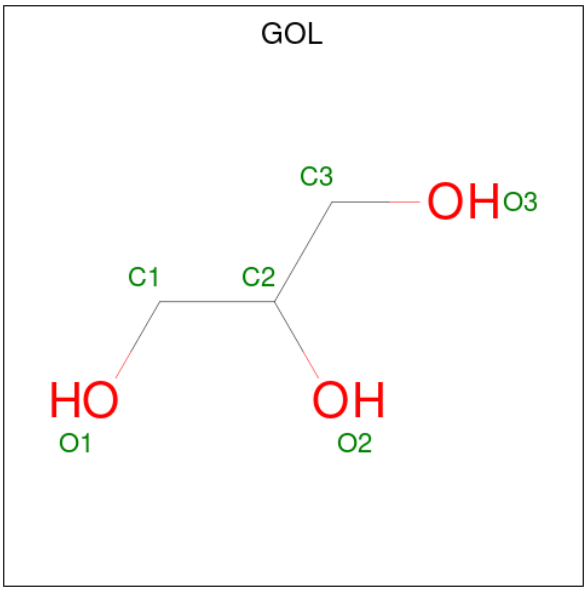
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	I	1	10	7	3	0	0
			Total	C	N		
3	L	1	10	7	3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

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

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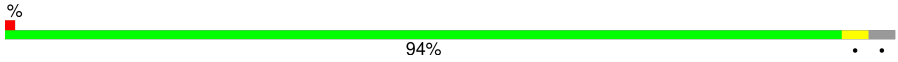
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	J	83	83	83	0	0
			Total	O		
6	K	58	58	58	0	0
			Total	O		
6	L	67	67	67	0	0

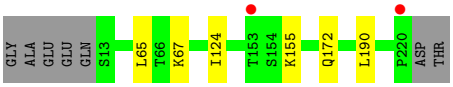
3 Residue-property plots (i)

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

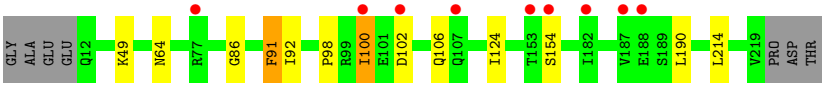
Chain A:





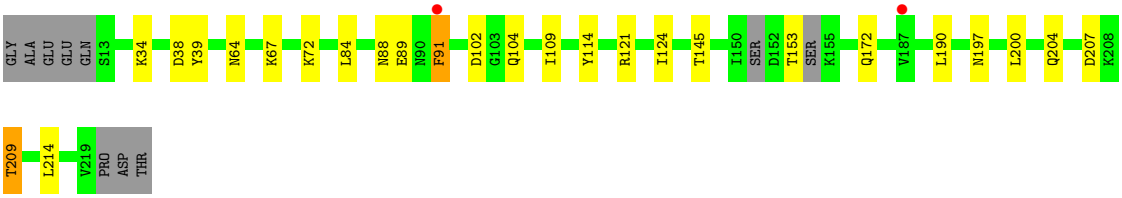
• Molecule 1: ANCILLARY PROTEIN 2

Chain B:



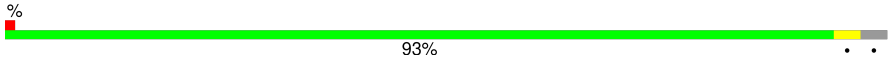
• Molecule 1: ANCILLARY PROTEIN 2

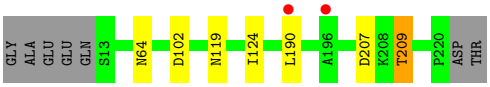
Chain C:



• Molecule 1: ANCILLARY PROTEIN 2

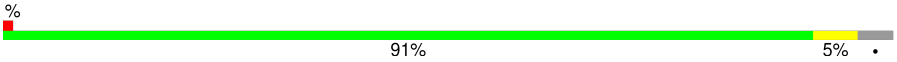
Chain D:

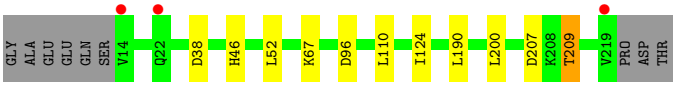




• Molecule 1: ANCILLARY PROTEIN 2

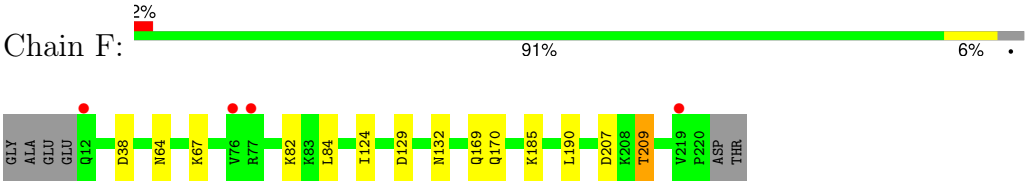
Chain E:





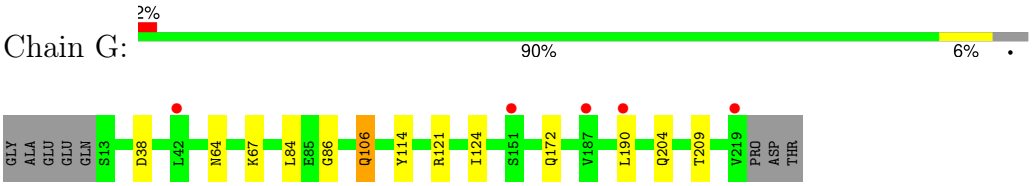
• Molecule 1: ANCILLARY PROTEIN 2

Chain F:



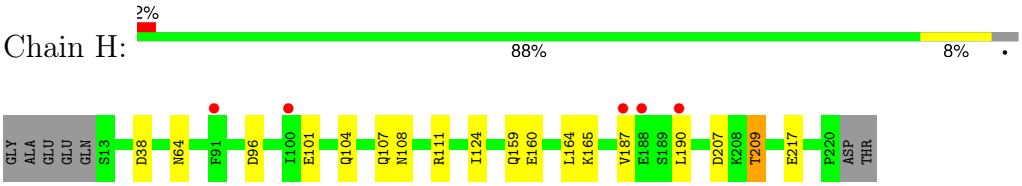
• Molecule 1: ANCILLARY PROTEIN 2

Chain G:



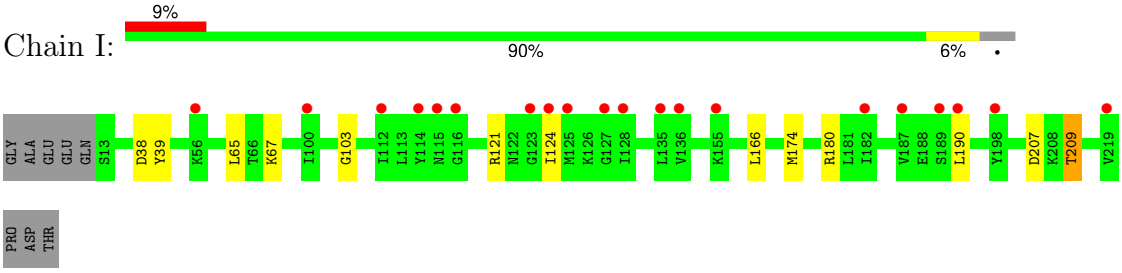
• Molecule 1: ANCILLARY PROTEIN 2

Chain H:



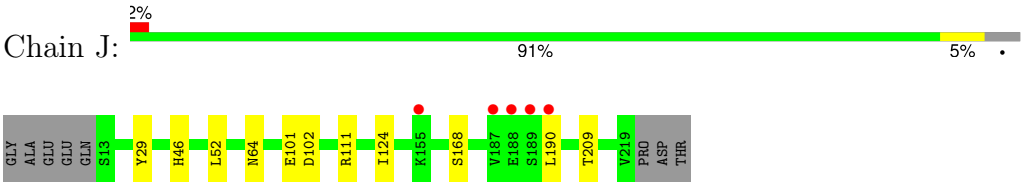
• Molecule 1: ANCILLARY PROTEIN 2

Chain I:



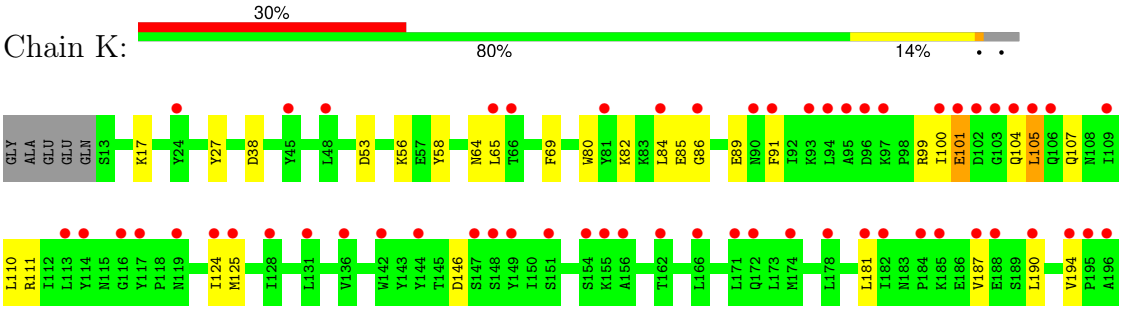
• Molecule 1: ANCILLARY PROTEIN 2

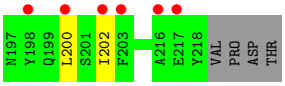
Chain J:



• Molecule 1: ANCILLARY PROTEIN 2

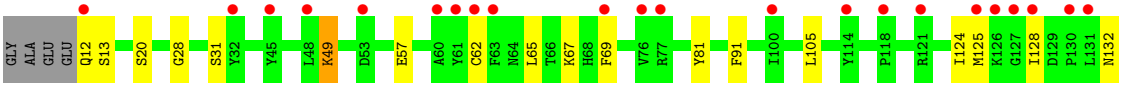
Chain K:

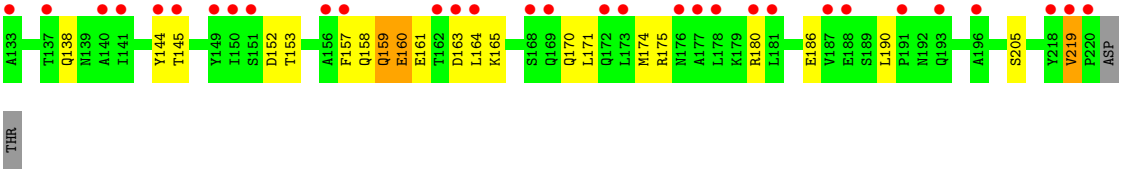




• Molecule 1: ANCILLARY PROTEIN 2

Chain L:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	9251 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)	0.34 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, SPD, CL, GOL

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 (i)

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.

All (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
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
1:A:155:LYS:HE2	1:K:104:GLN:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:ILE:HD11	1:E:190:LEU:HD11	1.87	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:K:125:MET:CE	1:K:181:LEU:HD11	2.37	0.54
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:I:166:LEU:HD22	1:I:174:MET:HE1	1.95	0.48
1:K:86:GLY:HA2	1:K:202:ILE:HG13	1.94	0.48
1:K:125:MET:HE1	1:K:181:LEU:HD11	1.94	0.48
1:L:132:ASN:HD22	1:L:170:GLN:HE21	1.61	0.48
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 (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%)	29	23
1	C	202/215 (94%)	198 (98%)	3 (2%)	1 (0%)	29	23
1	D	208/215 (97%)	203 (98%)	4 (2%)	1 (0%)	29	23
1	E	205/215 (95%)	202 (98%)	3 (2%)	0	100	100
1	F	208/215 (97%)	204 (98%)	3 (1%)	1 (0%)	29	23
1	G	206/215 (96%)	199 (97%)	6 (3%)	1 (0%)	29	23
1	H	208/215 (97%)	202 (97%)	5 (2%)	1 (0%)	29	23
1	I	206/215 (96%)	199 (97%)	7 (3%)	0	100	100
1	J	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	29	23
1	K	204/215 (95%)	189 (93%)	13 (6%)	2 (1%)	15	9
1	L	208/215 (97%)	195 (94%)	12 (6%)	1 (0%)	29	23
All	All	2476/2580 (96%)	2396 (97%)	70 (3%)	10 (0%)	34	30

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 (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	194/197 (98%)	194 (100%)	0	100	100
1	B	192/197 (98%)	188 (98%)	4 (2%)	53	57
1	C	192/197 (98%)	184 (96%)	8 (4%)	30	27
1	D	194/197 (98%)	191 (98%)	3 (2%)	65	69
1	E	191/197 (97%)	187 (98%)	4 (2%)	53	57
1	F	194/197 (98%)	192 (99%)	2 (1%)	76	81
1	G	192/197 (98%)	187 (97%)	5 (3%)	46	48
1	H	194/197 (98%)	189 (97%)	5 (3%)	46	48
1	I	192/197 (98%)	189 (98%)	3 (2%)	62	67
1	J	192/197 (98%)	188 (98%)	4 (2%)	53	57
1	K	188/197 (95%)	182 (97%)	6 (3%)	39	38
1	L	194/197 (98%)	186 (96%)	8 (4%)	30	28
All	All	2309/2364 (98%)	2257 (98%)	52 (2%)	53	53

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	49	LYS

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Mol	Chain	Res	Type
1	B	91	PHE
1	B	100	ILE
1	B	102	ASP
1	C	38	ASP
1	C	91[A]	PHE
1	C	91[B]	PHE
1	C	102	ASP
1	C	153	THR
1	C	172[A]	GLN
1	C	172[B]	GLN
1	C	209	THR
1	D	102	ASP
1	D	119	ASN
1	D	209	THR
1	E	38	ASP
1	E	52	LEU
1	E	96	ASP
1	E	209	THR
1	F	38	ASP
1	F	209	THR
1	G	38	ASP
1	G	106	GLN
1	G	172	GLN
1	G	209[A]	THR
1	G	209[B]	THR
1	H	38	ASP
1	H	96	ASP
1	H	101	GLU
1	H	159	GLN
1	H	209	THR
1	I	38	ASP
1	I	121	ARG
1	I	209	THR
1	J	52	LEU
1	J	101	GLU
1	J	168	SER
1	J	209	THR
1	K	38	ASP
1	K	85	GLU
1	K	89	GLU
1	K	101	GLU
1	K	105	LEU

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Mol	Chain	Res	Type
1	K	146	ASP
1	L	13	SER
1	L	20	SER
1	L	49	LYS
1	L	152	ASP
1	L	153	THR
1	L	159	GLN
1	L	160	GLU
1	L	163	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	192	ASN
1	B	18	GLN
1	B	119	ASN
1	C	18	GLN
1	C	46	HIS
1	C	88	ASN
1	C	104	GLN
1	C	106	GLN
1	C	204	GLN
1	D	18	GLN
1	D	158	GLN
1	E	46	HIS
1	E	204	GLN
1	F	18	GLN
1	F	104	GLN
1	F	170	GLN
1	F	204	GLN
1	G	204	GLN
1	H	18	GLN
1	H	108	ASN
1	H	119	ASN
1	I	18	GLN
1	J	46	HIS
1	K	18	GLN
1	K	64	ASN
1	K	107	GLN
1	L	18	GLN
1	L	138	GLN

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Mol	Chain	Res	Type
1	L	159	GLN
1	L	170	GLN
1	L	172	GLN
1	L	204	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 monosaccharides 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	0.70	0	8,8,8	0.73	0
4	PO4	F	1222	-	4,4,4	2.22	2 (50%)	6,6,6	0.43	0
3	SPD	G	1220	1	9,9,9	0.88	0	8,8,8	0.59	0
3	SPD	F	1223	1	9,9,9	0.72	0	8,8,8	1.11	1 (12%)
4	PO4	B	1220	-	4,4,4	2.23	4 (100%)	6,6,6	0.41	0
4	PO4	C	1222	-	4,4,4	1.98	1 (25%)	6,6,6	0.62	0
5	GOL	L	1222	-	5,5,5	0.11	0	5,5,5	0.35	0
5	GOL	C	1221	-	5,5,5	0.20	0	5,5,5	0.37	0
3	SPD	L	1223	1	9,9,9	0.70	0	8,8,8	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	I	1220	-	5,5,5	0.12	0	5,5,5	0.52	0
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%)

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	-	2/7/7/7	-
3	SPD	G	1220	1	-	4/7/7/7	-
3	SPD	F	1223	1	-	0/7/7/7	-
5	GOL	L	1222	-	-	0/4/4/4	-
5	GOL	C	1221	-	-	0/4/4/4	-
3	SPD	L	1223	1	-	3/7/7/7	-
5	GOL	I	1220	-	-	0/4/4/4	-
3	SPD	I	1221	1	-	3/7/7/7	-
3	SPD	C	1223	1	-	2/7/7/7	-

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(^{o})	Ideal(^{o})
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	A	1223	SPD	3	0
3	G	1220	SPD	2	0
3	F	1223	SPD	2	0
5	L	1222	GOL	1	0
5	C	1221	GOL	3	0
3	L	1223	SPD	4	0
5	I	1220	GOL	1	0
3	I	1221	SPD	2	0
3	C	1223	SPD	1	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	81	22, 37, 65, 88	0
1	B	208/215 (96%)	0.32	9 (4%)	35	34	21, 47, 87, 100	0
1	C	205/215 (95%)	0.01	2 (0%)	82	81	20, 37, 67, 88	0
1	D	208/215 (96%)	0.15	2 (0%)	82	81	23, 45, 76, 102	0
1	E	206/215 (95%)	0.25	3 (1%)	73	72	24, 46, 75, 83	0
1	F	209/215 (97%)	0.19	4 (1%)	66	65	27, 49, 81, 116	0
1	G	207/215 (96%)	0.15	5 (2%)	59	57	24, 43, 71, 87	0
1	H	208/215 (96%)	0.21	5 (2%)	59	57	24, 43, 77, 98	0
1	I	207/215 (96%)	0.63	20 (9%)	7	7	28, 58, 104, 121	0
1	J	207/215 (96%)	0.19	5 (2%)	59	57	22, 43, 76, 93	0
1	K	206/215 (95%)	1.70	64 (31%)	0	0	38, 62, 91, 112	0
1	L	209/215 (97%)	1.53	53 (25%)	0	0	31, 55, 87, 104	0
All	All	2488/2580 (96%)	0.45	174 (6%)	16	15	20, 47, 84, 121	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	187	VAL	12.7
1	K	105	LEU	8.9
1	K	187	VAL	8.8
1	L	150	ILE	7.2
1	K	100	ILE	7.2
1	L	162	THR	6.5
1	L	219	VAL	6.4
1	H	187	VAL	6.2
1	K	182	ILE	6.0
1	B	187	VAL	5.7
1	L	187	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
1	K	106	GLN	5.5
1	K	124	ILE	5.4
1	K	198	TYR	5.3
1	L	157	PHE	5.2
1	L	177	ALA	5.2
1	K	109	ILE	5.1
1	K	166	LEU	5.1
1	I	114	TYR	5.0
1	K	196	ALA	4.8
1	L	181	LEU	4.8
1	L	176	ASN	4.7
1	K	113	LEU	4.7
1	K	184	PRO	4.7
1	K	144	TYR	4.6
1	B	154	SER	4.5
1	K	155	LYS	4.5
1	I	187	VAL	4.5
1	L	140	ALA	4.3
1	L	180	ARG	4.3
1	G	187	VAL	4.3
1	K	194	VAL	4.2
1	K	174	MET	4.2
1	L	191	PRO	4.2
1	L	131	LEU	4.1
1	L	178	LEU	4.0
1	K	117	TYR	4.0
1	K	96	ASP	4.0
1	K	142	TRP	3.9
1	J	189	SER	3.9
1	L	220	PRO	3.8
1	L	144	TYR	3.8
1	K	178	LEU	3.8
1	L	114	TYR	3.7
1	I	125	MET	3.7
1	C	187	VAL	3.7
1	K	116	GLY	3.6
1	L	118	PRO	3.6
1	K	147	SER	3.6
1	L	169	GLN	3.6
1	K	86	GLY	3.5
1	L	77	ARG	3.5
1	K	90	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	202	ILE	3.4
1	K	200	LEU	3.4
1	L	164	LEU	3.4
1	L	127	GLY	3.4
1	K	188	GLU	3.4
1	K	149	TYR	3.3
1	L	149	TYR	3.3
1	K	103	GLY	3.3
1	K	203	PHE	3.3
1	B	102	ASP	3.2
1	L	193	GLN	3.2
1	I	219	VAL	3.2
1	K	125	MET	3.2
1	K	101	GLU	3.2
1	K	94	LEU	3.2
1	L	125	MET	3.1
1	L	141	ILE	3.1
1	K	84	LEU	3.1
1	L	156	ALA	3.1
1	I	127	GLY	3.1
1	J	190	LEU	3.1
1	K	154	SER	3.1
1	I	128	ILE	3.1
1	L	168	SER	3.1
1	K	172	GLN	3.0
1	L	126	LYS	3.0
1	B	153	THR	3.0
1	K	216	ALA	3.0
1	L	128	ILE	3.0
1	A	220	PRO	2.9
1	L	130	PRO	2.9
1	K	162	THR	2.9
1	I	124	ILE	2.9
1	J	188	GLU	2.9
1	I	190	LEU	2.9
1	K	114	TYR	2.9
1	L	45	TYR	2.9
1	K	181	LEU	2.9
1	G	219	VAL	2.8
1	L	100	ILE	2.8
1	L	173	LEU	2.8
1	J	155	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	148	SER	2.8
1	L	151	SER	2.8
1	K	190	LEU	2.8
1	K	97	LYS	2.8
1	D	196	ALA	2.7
1	B	100	ILE	2.7
1	I	182	ILE	2.7
1	G	190	LEU	2.7
1	K	24	TYR	2.7
1	H	190	LEU	2.7
1	K	128	ILE	2.7
1	K	102	ASP	2.7
1	I	136	VAL	2.6
1	L	196	ALA	2.6
1	B	107	GLN	2.6
1	H	188	GLU	2.6
1	K	171	LEU	2.6
1	I	112	ILE	2.6
1	K	48	LEU	2.6
1	G	151	SER	2.6
1	K	65	LEU	2.6
1	L	53	ASP	2.5
1	L	145	THR	2.5
1	L	137	THR	2.5
1	K	91	PHE	2.5
1	L	60	ALA	2.5
1	F	219	VAL	2.5
1	K	195	PRO	2.5
1	K	95	ALA	2.5
1	I	116	GLY	2.4
1	L	32	TYR	2.4
1	K	104	GLN	2.4
1	E	219	VAL	2.3
1	B	77	ARG	2.3
1	L	12	GLN	2.3
1	H	91	PHE	2.3
1	K	136	VAL	2.3
1	L	163	ASP	2.3
1	K	185	LYS	2.3
1	L	218	TYR	2.3
1	I	135	LEU	2.3
1	E	14	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	77	ARG	2.3
1	I	115	ASN	2.3
1	L	172	GLN	2.3
1	C	91[A]	PHE	2.3
1	F	76	VAL	2.3
1	K	119	ASN	2.3
1	I	100	ILE	2.3
1	I	198	TYR	2.2
1	K	156	ALA	2.2
1	E	22	GLN	2.2
1	L	76	VAL	2.2
1	K	131	LEU	2.2
1	K	217	GLU	2.2
1	L	61	TYR	2.2
1	L	63	PHE	2.2
1	G	42	LEU	2.1
1	I	123	GLY	2.1
1	L	48	LEU	2.1
1	L	121	ARG	2.1
1	A	153	THR	2.1
1	B	182	ILE	2.1
1	L	188	GLU	2.1
1	I	155	LYS	2.1
1	K	66	THR	2.1
1	K	93	LYS	2.1
1	H	100	ILE	2.1
1	K	151	SER	2.1
1	F	12	GLN	2.1
1	I	56	LYS	2.1
1	K	81	TYR	2.1
1	B	188	GLU	2.0
1	L	133	ALA	2.0
1	K	45	TYR	2.0
1	L	62	CYS	2.0
1	L	69	PHE	2.0
1	I	189	SER	2.0
1	D	190	LEU	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 monosaccharides 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(Å^2)	Q<0.9
5	GOL	L	1222	6/6	0.63	0.17	66,69,72,72	0
2	CL	H	1223	1/1	0.78	0.14	79,79,79,79	0
2	CL	B	1221	1/1	0.79	0.26	78,78,78,78	0
4	PO4	F	1222	5/5	0.83	0.20	80,80,81,82	0
3	SPD	L	1223	10/10	0.84	0.25	40,45,48,51	0
4	PO4	B	1220	5/5	0.84	0.25	86,88,90,90	0
5	GOL	I	1220	6/6	0.85	0.19	59,71,73,74	0
5	GOL	C	1221	6/6	0.85	0.17	36,51,55,56	0
2	CL	H	1222	1/1	0.90	0.12	82,82,82,82	0
2	CL	A	1222	1/1	0.92	0.16	72,72,72,72	0
2	CL	L	1224	1/1	0.94	0.07	79,79,79,79	0
2	CL	E	1220	1/1	0.95	0.18	69,69,69,69	0
3	SPD	C	1223	10/10	0.95	0.14	23,28,31,33	0
3	SPD	F	1223	10/10	0.95	0.15	23,30,34,36	0
2	CL	B	1222	1/1	0.96	0.23	58,58,58,58	0
2	CL	L	1221	1/1	0.97	0.10	40,40,40,40	0
4	PO4	C	1222	5/5	0.97	0.13	52,54,57,58	0
2	CL	G	1221	1/1	0.97	0.21	56,56,56,56	0
3	SPD	G	1220	10/10	0.97	0.16	29,32,33,33	0
3	SPD	I	1221	10/10	0.97	0.14	24,28,36,40	0
3	SPD	A	1223	10/10	0.97	0.16	22,25,28,33	0
2	CL	F	1221	1/1	0.98	0.12	37,37,37,37	0
2	CL	H	1221	1/1	0.99	0.10	33,33,33,33	0
2	CL	J	1220	1/1	0.99	0.14	31,31,31,31	0
2	CL	C	1220	1/1	1.00	0.10	29,29,29,29	0
2	CL	A	1221	1/1	1.00	0.10	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.