



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:18 PM 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

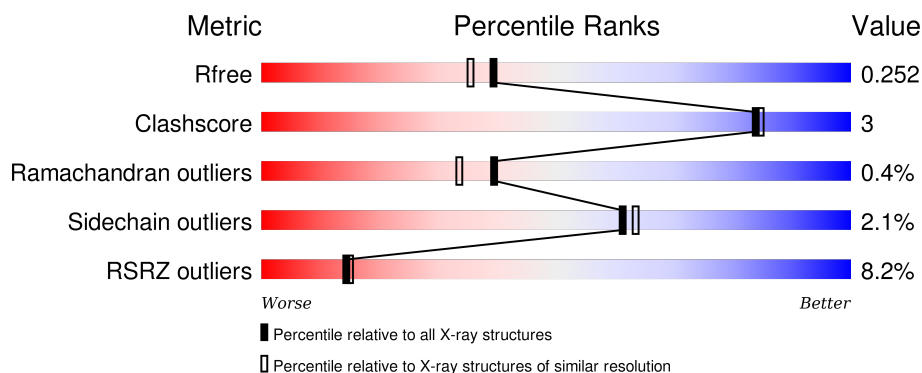
1 Overall quality at a glance i

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 style="width: 5%;"></div> <div>5%</div> </div>
1	C	215	<div> <div style="width: 83%;"></div> <div>83%</div> <div style="width: 11%;"></div> <div>11%</div> <div style="width: 5%;"></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 style="width: 5%;"></div> <div>5%</div> </div>

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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
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 [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
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).

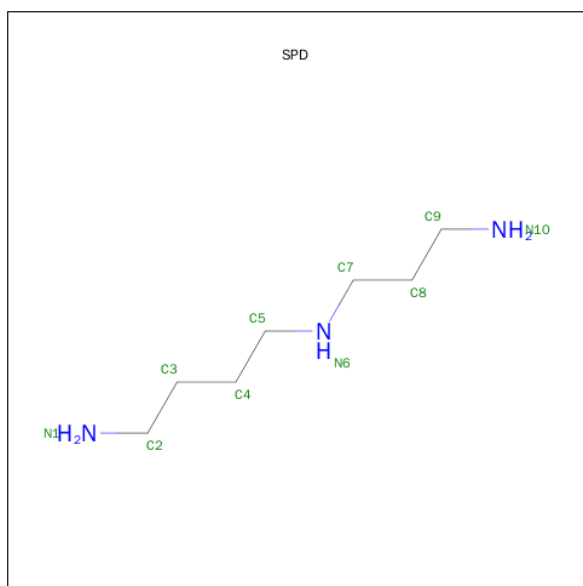
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Cl	0	0
			1	1		
2	J	1	Total	Cl	0	0
			1	1		

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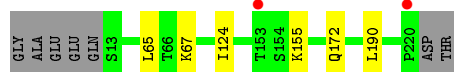
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	83	Total 83	O 83	0	0
6	K	58	Total 58	O 58	0	0
6	L	67	Total 67	O 67	0	0

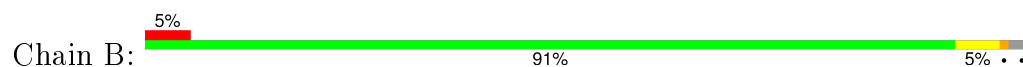
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

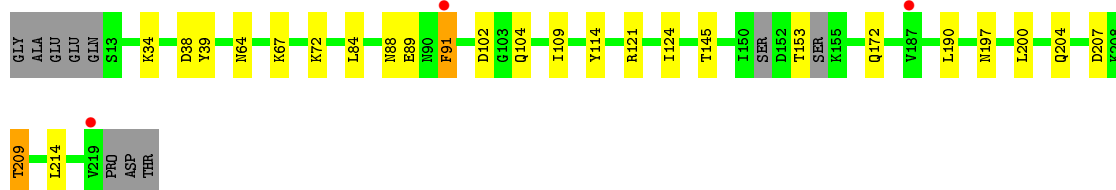
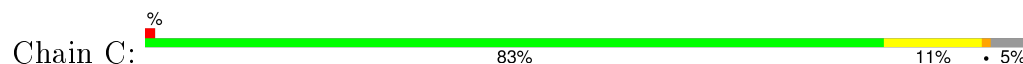
• Molecule 1: ANCILLARY PROTEIN 2



• Molecule 1: ANCILLARY PROTEIN 2



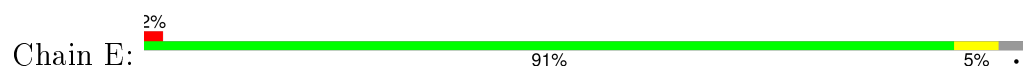
• Molecule 1: ANCILLARY PROTEIN 2



• Molecule 1: ANCILLARY PROTEIN 2



• Molecule 1: ANCILLARY PROTEIN 2

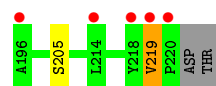


[illegible][illegible]

Gly
ALA
Glu
Gln
Gln
S13
D88
N64
F91
D96
I100
E101
Q104
Q107
N108
R111
R121
I124
Q159
E160
L164
K165
V187
E188
S189
L190
D207
K208
T209
E217
P220
ASP
TSP

GLY	ALA	GLU	GLU	GLN	S13	Y29	H46	L52	N64	E101	D102	R111	I124	K155	S168	V187	E188	S189	L190	T209	V219	PRO	ASP	THR
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L105	L106	L107	L108	L109	L110	L111	L112	L113	L114	L115	L116	L117	L118	L119	L120	L121	L122	L123	L124	L125	L126	L127	L128	L129	L130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	L175	L176	L177	L178	L179	L180	L181	L182	L183	L184	L185	L186	L187	L188	L189	L190	L191	L192	L193	L194	L195	L196	L197	L198	L199	L200	L201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L61
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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	9228 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 , 56.1	EDS
Estimated twinning fraction	0.024 for -h,-k,l 0.031 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 180592 reflections	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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.

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:O	1:L:219:VAL:HG12	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:K:111:ARG:HB3	1:K:187:VAL:HG11	1.91	0.50
1:A:124:ILE:HD11	1:A:190:LEU:HD11	1.91	0.50
1:L:67:LYS:O	3:L:1223:SPD:C5	2.60	0.49
6:I:2036:HOH:O	1:J:46:HIS:HE1	1.93	0.49
1:D:124:ILE:HD11	1:D:190:LEU:HD11	1.94	0.49
1:L:132:ASN:HD22	1:L:170:GLN:NE2	2.10	0.49
1:D:207:ASP:OD1	1:D:209:THR:HB	2.12	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	1.95	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:L:171:LEU:HD21	1:L:175:ARG:CZ	2.47	0.45
1:E:67:LYS:O	3:F:1223:SPD:H71	2.17	0.45
1:L:28:GLY:HA3	1:L:81:TYR:CE1	2.52	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:F:207:ASP:OD1	1:F:209:THR:HB	2.17	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:H:108:ASN:HA	1:H:111:ARG:NH1	2.32	0.44
1:A:65:LEU:O	3:A:1223:SPD:H51	2.17	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:L:12:GLN:HB2	1:L:31:SER:HB2	2.01	0.42
1:B:86:GLY:O	1:B:106:GLN:HG3	2.20	0.42
1:B:92:ILE:HG12	1:B:100:ILE:HD11	2.01	0.42
1:L:164:LEU:O	1:L:165:LYS:HG2	2.20	0.42
1:E:110:LEU:HG	1:E:200:LEU:HB2	2.02	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:K:56:LYS:HD3	1:K:58:TYR:CZ	2.56	0.41
1:F:82:LYS:O	1:F:84:LEU:HD22	2.20	0.41
1:K:69:PHE:CE1	3:L:1223:SPD:H91	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:TYR:OH	5:I:1220:GOL:H32	2.20	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:K:17:LYS:HD2	1:K:27:TYR:CZ	2.56	0.40
1:A:67:LYS:O	3:A:1223:SPD:H52	2.21	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%)	34	26
1	C	202/215 (94%)	198 (98%)	3 (2%)	1 (0%)	34	26
1	D	208/215 (97%)	203 (98%)	4 (2%)	1 (0%)	34	26
1	E	205/215 (95%)	202 (98%)	3 (2%)	0	100	100
1	F	208/215 (97%)	204 (98%)	3 (1%)	1 (0%)	34	26
1	G	206/215 (96%)	199 (97%)	6 (3%)	1 (0%)	34	26
1	H	208/215 (97%)	202 (97%)	5 (2%)	1 (0%)	34	26
1	I	206/215 (96%)	199 (97%)	7 (3%)	0	100	100
1	J	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	34	26
1	K	204/215 (95%)	189 (93%)	13 (6%)	2 (1%)	19	11
1	L	208/215 (97%)	195 (94%)	12 (6%)	1 (0%)	34	26
All	All	2476/2580 (96%)	2396 (97%)	70 (3%)	10 (0%)	39	33

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%)	194 (100%)	0	100	100
1	B	192/197 (98%)	188 (98%)	4 (2%)	61	63
1	C	192/197 (98%)	184 (96%)	8 (4%)	36	31
1	D	194/197 (98%)	191 (98%)	3 (2%)	72	75
1	E	191/197 (97%)	187 (98%)	4 (2%)	61	63
1	F	194/197 (98%)	192 (99%)	2 (1%)	82	85
1	G	192/197 (98%)	187 (97%)	5 (3%)	54	54
1	H	194/197 (98%)	189 (97%)	5 (3%)	54	54
1	I	192/197 (98%)	189 (98%)	3 (2%)	70	73
1	J	192/197 (98%)	188 (98%)	4 (2%)	61	63
1	K	188/197 (95%)	182 (97%)	6 (3%)	46	44
1	L	194/197 (98%)	186 (96%)	8 (4%)	37	32
All	All	2309/2364 (98%)	2257 (98%)	52 (2%)	61	60

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

Some 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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.72	0	8,8,8	0.77	0
4	PO4	B	1220	-	4,4,4	1.80	0	6,6,6	0.27	0
5	GOL	C	1221	-	5,5,5	0.21	0	5,5,5	0.41	0
4	PO4	C	1222	-	4,4,4	1.70	0	6,6,6	0.28	0
3	SPD	C	1223	1	9,9,9	0.64	0	8,8,8	1.03	1 (12%)
4	PO4	F	1222	-	4,4,4	1.79	1 (25%)	6,6,6	0.26	0
3	SPD	F	1223	1	9,9,9	0.73	0	8,8,8	1.19	1 (12%)
3	SPD	G	1220	1	9,9,9	0.90	0	8,8,8	0.64	0
5	GOL	I	1220	-	5,5,5	0.17	0	5,5,5	0.44	0

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	0.68	0	8,8,8	0.74	0
5	GOL	L	1222	-	5,5,5	0.12	0	5,5,5	0.43	0
3	SPD	L	1223	1	9,9,9	0.71	0	8,8,8	0.80	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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1222	PO4	P-O2	2.03	1.60	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1223	SPD	C8-C7-N6	-3.14	104.12	111.96
3	C	1223	SPD	C8-C7-N6	-2.59	105.49	111.96

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 ⓘ

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	2 (0%) 84 84	22, 37, 65, 88	0
1	B	208/215 (96%)	0.40	11 (5%) 30 32	21, 47, 87, 100	0
1	C	205/215 (95%)	0.07	3 (1%) 76 77	20, 37, 67, 88	0
1	D	208/215 (96%)	0.22	2 (0%) 84 84	23, 45, 76, 102	0
1	E	206/215 (95%)	0.33	4 (1%) 70 70	24, 46, 75, 83	0
1	F	209/215 (97%)	0.26	6 (2%) 55 56	27, 49, 81, 116	0
1	G	207/215 (96%)	0.22	6 (2%) 55 56	24, 43, 71, 87	0
1	H	208/215 (96%)	0.28	6 (2%) 55 56	24, 43, 77, 98	0
1	I	207/215 (96%)	0.71	24 (11%) 6 7	28, 58, 104, 121	0
1	J	207/215 (96%)	0.26	6 (2%) 55 56	22, 43, 76, 93	0
1	K	206/215 (95%)	1.83	72 (34%) 0 1	38, 62, 91, 112	0
1	L	209/215 (97%)	1.66	63 (30%) 1 1	31, 55, 87, 104	0
All	All	2488/2580 (96%)	0.53	205 (8%) 14 15	20, 47, 84, 121	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	187	VAL	13.5
1	K	187	VAL	9.6
1	K	105	LEU	9.4
1	K	100	ILE	7.9
1	L	150	ILE	7.7
1	L	219	VAL	6.9
1	L	162	THR	6.7
1	H	187	VAL	6.6
1	K	182	ILE	6.4
1	B	187	VAL	6.3
1	L	187	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	K	124	ILE	5.7
1	L	177	ALA	5.7
1	L	157	PHE	5.6
1	K	106	GLN	5.6
1	K	198	TYR	5.6
1	K	109	ILE	5.4
1	K	166	LEU	5.4
1	L	181	LEU	5.2
1	K	196	ALA	5.2
1	I	114	TYR	5.2
1	K	113	LEU	5.0
1	K	184	PRO	5.0
1	L	176	ASN	5.0
1	B	154	SER	4.8
1	L	140	ALA	4.7
1	I	187	VAL	4.7
1	K	144	TYR	4.7
1	G	187	VAL	4.7
1	K	194	VAL	4.6
1	K	155	LYS	4.6
1	L	180	ARG	4.5
1	L	191	PRO	4.4
1	K	174	MET	4.4
1	L	131	LEU	4.4
1	L	178	LEU	4.3
1	K	117	TYR	4.2
1	K	96	ASP	4.2
1	J	189	SER	4.1
1	K	142	TRP	4.1
1	K	178	LEU	4.1
1	L	220	PRO	4.1
1	C	187	VAL	4.0
1	L	144	TYR	4.0
1	I	125	MET	3.9
1	L	114	TYR	3.9
1	K	116	GLY	3.8
1	K	86	GLY	3.8
1	K	147	SER	3.8
1	L	118	PRO	3.7
1	L	169	GLN	3.7
1	K	90	ASN	3.7
1	L	77	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	L	164	LEU	3.7
1	L	127	GLY	3.6
1	K	202	ILE	3.6
1	K	188	GLU	3.6
1	K	200	LEU	3.5
1	K	103	GLY	3.5
1	K	149	TYR	3.5
1	L	149	TYR	3.4
1	K	125	MET	3.4
1	K	203	PHE	3.4
1	L	193	GLN	3.4
1	L	141	ILE	3.4
1	I	219	VAL	3.4
1	B	102	ASP	3.4
1	I	128	ILE	3.4
1	K	84	LEU	3.3
1	K	94	LEU	3.3
1	L	156	ALA	3.3
1	J	190	LEU	3.3
1	L	125	MET	3.3
1	L	168	SER	3.3
1	K	101	GLU	3.3
1	B	153	THR	3.3
1	I	127	GLY	3.2
1	K	216	ALA	3.2
1	K	172	GLN	3.2
1	K	154	SER	3.2
1	L	128	ILE	3.2
1	L	126	LYS	3.2
1	L	130	PRO	3.1
1	I	124	ILE	3.1
1	K	181	LEU	3.1
1	K	162	THR	3.1
1	A	220	PRO	3.1
1	L	100	ILE	3.1
1	G	219	VAL	3.1
1	L	45	TYR	3.0
1	L	151	SER	3.0
1	I	190	LEU	3.0
1	K	148	SER	3.0
1	L	173	LEU	3.0
1	K	114	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	190	LEU	3.0
1	J	188	GLU	2.9
1	K	128	ILE	2.9
1	K	97	LYS	2.9
1	B	100	ILE	2.9
1	G	190	LEU	2.9
1	D	196	ALA	2.9
1	I	182	ILE	2.9
1	L	196	ALA	2.9
1	K	171	LEU	2.9
1	K	24	TYR	2.9
1	L	53	ASP	2.9
1	J	155	LYS	2.8
1	H	190	LEU	2.8
1	I	136	VAL	2.8
1	K	65	LEU	2.8
1	K	102	ASP	2.8
1	H	188	GLU	2.8
1	K	48	LEU	2.8
1	L	137	THR	2.7
1	K	91	PHE	2.7
1	G	151	SER	2.7
1	I	112	ILE	2.7
1	L	60	ALA	2.7
1	L	145	THR	2.7
1	B	107	GLN	2.7
1	F	219	VAL	2.7
1	K	95	ALA	2.6
1	K	195	PRO	2.6
1	I	116	GLY	2.6
1	L	163	ASP	2.5
1	K	104	GLN	2.5
1	L	32	TYR	2.5
1	K	136	VAL	2.5
1	E	219	VAL	2.5
1	L	76	VAL	2.5
1	K	156	ALA	2.5
1	H	91	PHE	2.5
1	L	12	GLN	2.5
1	E	14	VAL	2.5
1	B	77	ARG	2.4
1	I	115	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	185	LYS	2.4
1	L	172	GLN	2.4
1	C	91[A]	PHE	2.4
1	I	198	TYR	2.4
1	L	218	TYR	2.4
1	F	76	VAL	2.4
1	I	135	LEU	2.4
1	K	131	LEU	2.4
1	F	77	ARG	2.4
1	I	100	ILE	2.4
1	L	61	TYR	2.3
1	L	63	PHE	2.3
1	K	119	ASN	2.3
1	E	22	GLN	2.3
1	L	133	ALA	2.3
1	B	182	ILE	2.3
1	K	66	THR	2.3
1	L	121	ARG	2.3
1	G	42	LEU	2.3
1	A	153	THR	2.2
1	H	100	ILE	2.2
1	I	123	GLY	2.2
1	D	190	LEU	2.2
1	L	48	LEU	2.2
1	K	217	GLU	2.2
1	L	188	GLU	2.2
1	K	93	LYS	2.2
1	K	45	TYR	2.2
1	K	81	TYR	2.2
1	L	69	PHE	2.2
1	L	117	TYR	2.2
1	K	115	ASN	2.2
1	L	62	CYS	2.2
1	F	12	GLN	2.1
1	F	220	PRO	2.1
1	K	112	ILE	2.1
1	K	151	SER	2.1
1	H	121	ARG	2.1
1	I	56	LYS	2.1
1	L	134	ILE	2.1
1	L	171	LEU	2.1
1	K	67	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	155	LYS	2.1
1	L	113	LEU	2.1
1	I	189	SER	2.1
1	G	76	VAL	2.1
1	L	214	LEU	2.1
1	B	101	GLU	2.1
1	B	188	GLU	2.1
1	L	115	ASN	2.1
1	F	187	VAL	2.1
1	K	50	VAL	2.1
1	L	182	ILE	2.0
1	K	111	ARG	2.0
1	E	172	GLN	2.0
1	I	166	LEU	2.0
1	I	168	SER	2.0
1	L	174	MET	2.0
1	L	120	ASP	2.0
1	C	219	VAL	2.0
1	I	153	THR	2.0
1	J	219	VAL	2.0
1	K	87	THR	2.0
1	L	22	GLN	2.0
1	I	197	ASN	2.0
1	B	91	PHE	2.0
1	K	25	PRO	2.0
1	K	189	SER	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 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(\AA^2)	Q<0.9
2	CL	B	1221	1/1	0.80	0.26	5.92	78,78,78,78	0
3	SPD	A	1223	10/10	0.97	0.16	3.73	22,25,28,33	0
5	GOL	I	1220	6/6	0.84	0.19	3.38	59,71,73,74	0
4	PO4	B	1220	5/5	0.84	0.26	3.38	86,88,90,90	0
4	PO4	F	1222	5/5	0.83	0.20	3.36	80,80,81,82	0
3	SPD	G	1220	10/10	0.97	0.16	2.22	29,32,33,33	0
3	SPD	C	1223	10/10	0.96	0.15	1.63	23,28,31,33	0
3	SPD	F	1223	10/10	0.95	0.15	1.62	23,30,34,36	0
3	SPD	I	1221	10/10	0.97	0.14	1.06	24,28,36,40	0
3	SPD	L	1223	10/10	0.84	0.25	0.92	40,45,48,51	0
4	PO4	C	1222	5/5	0.97	0.14	0.79	52,54,57,58	0
2	CL	A	1222	1/1	0.92	0.16	0.67	72,72,72,72	0
5	GOL	C	1221	6/6	0.85	0.17	0.37	36,51,55,56	0
2	CL	J	1220	1/1	0.99	0.14	0.19	31,31,31,31	0
2	CL	H	1223	1/1	0.78	0.13	0.13	79,79,79,79	0
2	CL	F	1221	1/1	0.98	0.12	-1.01	37,37,37,37	0
2	CL	C	1220	1/1	1.00	0.10	-1.45	29,29,29,29	0
2	CL	H	1221	1/1	0.99	0.10	-1.72	33,33,33,33	0
2	CL	A	1221	1/1	1.00	0.10	-2.20	27,27,27,27	0
2	CL	L	1221	1/1	0.97	0.11	-2.55	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	0.93	0.07	-	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.