



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:52 AM UTC

PDB ID : 2XJO / pdb_00002xjo
Title : Crystal structure of Streptococcus suis Dpr with nickel
Authors : Haikarainen, T.; Thanassoulas, A.; Stavros, P.; Nounesis, G.; Haataja, S.;
Papageorgiou, A.C.
Deposited on : 2010-07-06
Resolution : 2.10 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

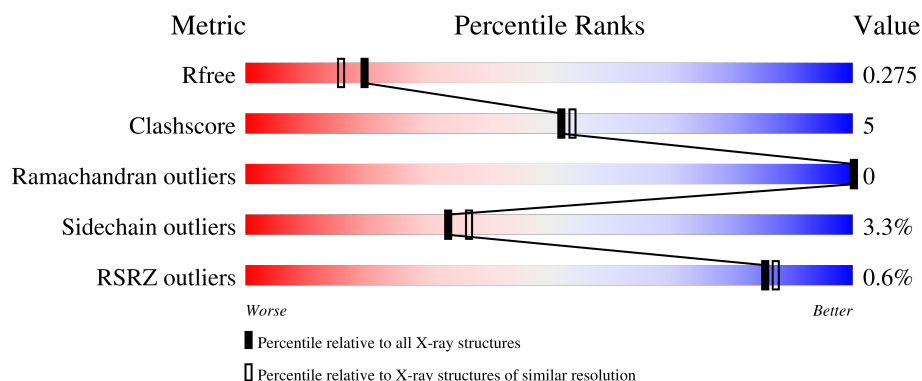
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	165	80% 11% 9%
1	B	165	76% 15% 8%
1	C	165	77% 14% 9%
1	D	165	81% 12% 8%
1	E	165	81% 11% 8%

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Mol	Chain	Length	Quality of chain
1	F	165	% 85% 7% 8%
1	G	165	80% 10% 10%
1	H	165	79% 12% 8%
1	I	165	% 72% 18% • 8%
1	J	165	% 80% 10% • 8%
1	K	165	81% 10% • 8%
1	L	165	% 80% 11% • 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15560 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 DNA PROTECTION DURING STARVATION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	2	0
			1218	775	200	236	7			
1	B	151	Total	C	N	O	S	0	3	0
			1223	779	201	236	7			
1	C	150	Total	C	N	O	S	0	0	0
			1197	762	197	232	6			
1	D	152	Total	C	N	O	S	0	5	0
			1259	798	208	246	7			
1	E	151	Total	C	N	O	S	0	3	0
			1221	777	200	238	6			
1	F	151	Total	C	N	O	S	0	3	0
			1235	785	202	242	6			
1	G	149	Total	C	N	O	S	0	4	0
			1227	778	201	242	6			
1	H	151	Total	C	N	O	S	0	2	0
			1216	775	200	235	6			
1	I	151	Total	C	N	O	S	0	3	0
			1212	772	202	232	6			
1	J	151	Total	C	N	O	S	0	3	0
			1223	778	200	239	6			
1	K	152	Total	C	N	O	S	0	6	0
			1252	793	206	247	6			
1	L	152	Total	C	N	O	S	0	6	0
			1243	789	203	245	6			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

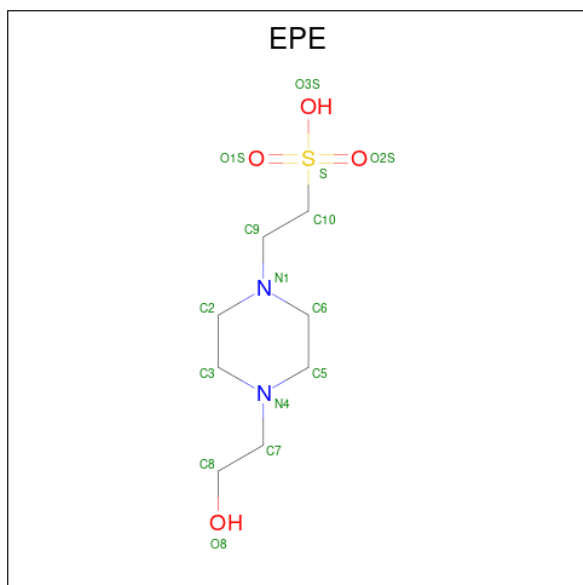
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		
2	B	1	Total	Ni	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Ni	0	0
			1	1		
2	D	1	Total	Ni	0	0
			1	1		
2	E	1	Total	Ni	0	0
			1	1		
2	F	1	Total	Ni	0	0
			1	1		
2	G	1	Total	Ni	0	0
			1	1		
2	H	1	Total	Ni	0	0
			1	1		
2	I	1	Total	Ni	0	0
			1	1		
2	J	1	Total	Ni	0	0
			1	1		
2	K	1	Total	Ni	0	0
			1	1		
2	L	1	Total	Ni	0	0
			1	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	K	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	F	2	Total	Ca	0	0
			2	2		
4	I	1	Total	Ca	0	0
			1	1		
4	J	1	Total	Ca	0	0
			1	1		
4	K	1	Total	Ca	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	E	1	Total	Cl	0	0
			1	1		
5	G	1	Total	Cl	0	0
			1	1		
5	I	1	Total	Cl	0	0
			1	1		
5	J	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

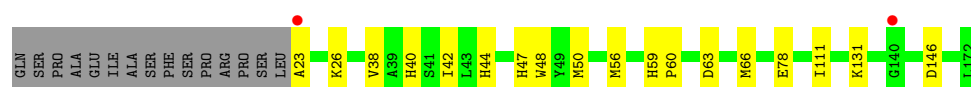
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	58	Total 58	O 58	0	0
6	B	92	Total 92	O 92	0	0
6	C	42	Total 42	O 42	0	0
6	D	96	Total 96	O 96	0	0
6	E	38	Total 38	O 38	0	0
6	F	79	Total 79	O 79	0	0
6	G	46	Total 46	O 46	0	0
6	H	48	Total 48	O 48	0	0
6	I	54	Total 54	O 54	0	0
6	J	61	Total 61	O 61	0	0
6	K	75	Total 75	O 75	0	0
6	L	60	Total 60	O 60	0	0

3 Residue-property plots

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.

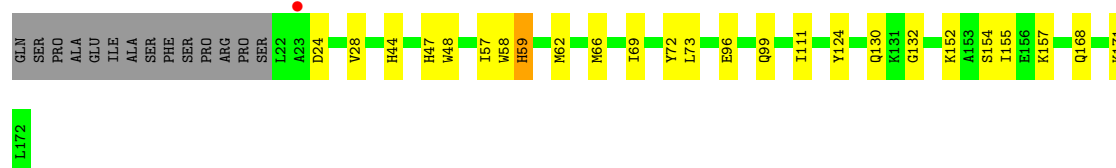
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain A: 



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain B: 



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain C: 



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain D: 



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain E: 



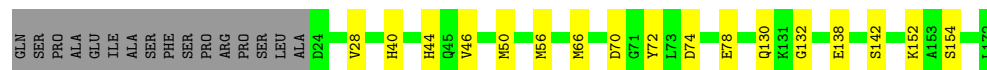
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain F: 



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain G: 



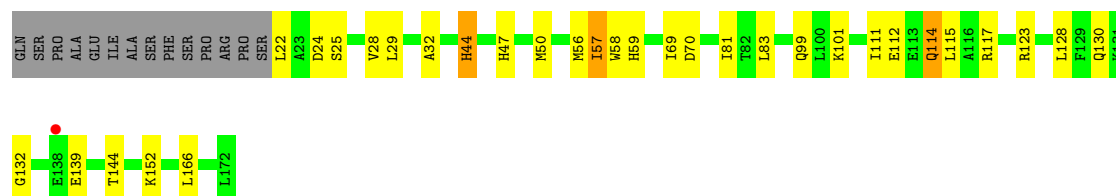
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain H: 



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain I: 



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain J: 



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain K: 



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.86Å 137.46Å 141.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.10) 98.9 (20.00-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.4.0078	Depositor
R, R_{free}	0.176 , 0.222 0.243 , 0.275	Depositor DCC
R_{free} test set	5940 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15560	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, CL, NI, CA

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	0.85	0/1243	0.95	0/1677
1	B	0.96	0/1252	0.97	4/1690 (0.2%)
1	C	0.82	0/1222	0.91	0/1651
1	D	0.96	0/1284	0.92	2/1732 (0.1%)
1	E	0.75	0/1250	0.91	1/1689 (0.1%)
1	F	0.93	0/1260	0.93	0/1701
1	G	0.78	0/1252	0.90	0/1690
1	H	0.84	0/1245	0.95	0/1681
1	I	0.86	0/1245	0.94	1/1682 (0.1%)
1	J	0.89	0/1252	0.93	0/1692
1	K	0.88	0/1285	0.94	0/1735
1	L	0.82	0/1280	0.94	0/1728
All	All	0.87	0/15070	0.93	8/20348 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	HIS	CA-C-N	-6.13	112.69	119.19
1	B	59	HIS	C-N-CA	-6.13	112.69	119.19
1	I	25	SER	N-CA-C	-6.03	104.62	111.07
1	B	24	ASP	N-CA-C	5.88	116.86	108.74
1	B	48	TRP	N-CA-C	5.79	117.68	111.36
1	E	48	TRP	N-CA-C	5.76	117.64	111.36
1	D	59	HIS	CA-C-N	-5.31	113.56	119.19
1	D	59	HIS	C-N-CA	-5.31	113.56	119.19

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	1218	0	1176	10	0
1	B	1223	0	1182	15	0
1	C	1197	0	1152	12	0
1	D	1259	0	1210	15	0
1	E	1221	0	1170	10	0
1	F	1235	0	1187	9	0
1	G	1227	0	1173	10	0
1	H	1216	0	1176	11	0
1	I	1212	0	1169	22	0
1	J	1223	0	1169	13	0
1	K	1252	0	1195	20	0
1	L	1243	0	1192	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	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	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	B	15	0	17	1	0
3	G	15	0	17	1	0
3	K	15	0	17	1	0
3	L	15	0	17	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	2	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
6	A	58	0	0	0	0
6	B	92	0	0	1	0
6	C	42	0	0	0	0
6	D	96	0	0	4	0
6	E	38	0	0	3	0
6	F	79	0	0	1	0
6	G	46	0	0	0	0
6	H	48	0	0	0	0
6	I	54	0	0	4	0
6	J	61	0	0	0	0
6	K	75	0	0	0	0
6	L	60	0	0	0	0
All	All	15560	0	14219	147	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 5.

All (147) 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:117[A]:ARG:HH11	1:K:117[A]:ARG:CG	1.55	1.16
1:K:117[A]:ARG:HG3	1:K:117[A]:ARG:NH1	1.52	1.04
1:C:130:GLN:NE2	1:C:152:LYS:HE3	1.82	0.95
1:C:130:GLN:HE21	1:C:152:LYS:HE3	1.32	0.94
1:L:21:SER:N	1:L:22:LEU:HA	1.86	0.88
1:H:130:GLN:NE2	1:H:152:LYS:HE3	1.89	0.87
1:K:117[A]:ARG:HH11	1:K:117[A]:ARG:HG3	0.70	0.86
1:L:130:GLN:HE21	1:L:152:LYS:HE3	1.40	0.85
1:J:114:GLN:HE21	1:J:114:GLN:HA	1.42	0.83
1:H:130:GLN:HE21	1:H:152:LYS:HE3	1.42	0.83
1:L:130:GLN:NE2	1:L:152:LYS:HE3	1.94	0.83
1:B:130:GLN:HE21	1:B:152:LYS:HE3	1.43	0.82
1:F:130:GLN:NE2	1:F:152:LYS:HE3	1.96	0.81
1:D:130:GLN:NE2	1:D:152:LYS:HE3	1.95	0.80
1:F:130:GLN:HE21	1:F:152:LYS:HE3	1.50	0.76
1:L:114:GLN:HE21	1:L:114:GLN:HA	1.50	0.76
1:D:130:GLN:HE21	1:D:152:LYS:HE3	1.50	0.75
1:K:114:GLN:HA	1:K:114:GLN:HE21	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLN:NE2	1:B:152:LYS:HE3	2.05	0.72
1:G:40:HIS:CE1	1:G:66:MET:HE3	2.26	0.71
1:A:23:ALA:HB3	1:A:26:LYS:HG3	1.73	0.70
1:F:24:ASP:HB3	1:F:135:VAL:HG11	1.73	0.69
1:E:72:TYR:OH	1:E:154[B]:SER:OG	2.11	0.68
1:B:168:GLN:HE21	1:B:171:LYS:NZ	1.91	0.68
1:K:117[A]:ARG:CG	1:K:117[A]:ARG:NH1	2.26	0.68
1:F:24:ASP:HB3	1:F:135:VAL:CG1	2.24	0.67
1:K:114:GLN:HE22	1:K:117[B]:ARG:NH2	1.93	0.67
1:B:157:LYS:HE3	1:L:78[B]:GLU:OE2	1.94	0.67
1:B:168:GLN:HE21	1:B:171:LYS:HZ1	1.42	0.65
1:K:114:GLN:HE22	1:K:117[B]:ARG:HH22	1.45	0.65
1:L:21:SER:HB3	1:L:23:ALA:H	1.62	0.64
1:D:110:THR:HA	6:D:2065:HOH:O	1.97	0.64
1:F:117:ARG:NH1	6:F:2048:HOH:O	2.31	0.63
1:I:112:GLU:HG3	6:I:2041:HOH:O	1.99	0.62
1:A:40:HIS:CE1	1:A:66[B]:MET:HE3	2.36	0.61
1:I:114:GLN:HE21	1:I:114:GLN:HA	1.66	0.60
1:A:78[B]:GLU:OE1	1:E:157:LYS:HE3	2.01	0.60
1:C:92:LYS:O	1:C:96:GLU:HG3	2.02	0.59
1:G:72:TYR:HH	1:G:154[A]:SER:HG	1.42	0.59
1:K:74:ASP:O	1:K:78[B]:GLU:HG3	2.01	0.59
1:I:130:GLN:NE2	1:I:152:LYS:HE3	2.19	0.58
1:J:130:GLN:HE21	1:J:152:LYS:HE3	1.67	0.58
1:E:32:ALA:HA	1:E:128:LEU:HD21	1.86	0.57
1:G:74:ASP:O	1:G:78[B]:GLU:HG3	2.04	0.57
1:D:130:GLN:NE2	6:D:2077:HOH:O	2.34	0.57
1:C:45:GLN:NE2	1:C:117:ARG:HH22	2.04	0.54
1:D:58:TRP:CH2	1:I:56:MET:HE3	2.42	0.54
1:I:123[A]:ARG:HD3	6:I:2044:HOH:O	2.07	0.54
1:E:117:ARG:NH1	6:E:2026:HOH:O	2.35	0.54
1:I:81:ILE:HD11	1:K:48:TRP:HB3	1.90	0.54
1:D:117[A]:ARG:O	1:D:117[A]:ARG:HD2	2.08	0.53
1:J:78:GLU:HA	1:J:81:ILE:HD12	1.91	0.53
1:K:28:VAL:HG11	1:K:132:GLY:HA2	1.91	0.52
1:F:134:ASP:O	1:F:138:GLU:HG3	2.10	0.52
1:C:47:HIS:CE1	1:C:59:HIS:CE1	2.98	0.52
1:D:74[B]:ASP:O	1:D:78[B]:GLU:HG3	2.10	0.52
1:E:117:ARG:NH2	6:E:2025:HOH:O	2.43	0.51
1:J:130:GLN:NE2	1:J:152:LYS:HE3	2.25	0.51
1:C:161:MET:HB3	1:L:56:MET:HE1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:MET:HE1	1:K:161:MET:HB3	1.93	0.51
1:J:114:GLN:HA	1:J:114:GLN:NE2	2.19	0.51
1:A:40:HIS:HE1	1:A:66[B]:MET:HE3	1.77	0.50
1:C:45:GLN:HE21	1:C:117:ARG:HH12	1.59	0.50
1:G:72:TYR:OH	1:G:154[A]:SER:OG	2.17	0.50
1:A:47:HIS:CE1	1:A:59:HIS:CE1	3.00	0.50
1:B:72:TYR:OH	1:B:154[A]:SER:OG	2.22	0.50
1:G:28:VAL:HG11	1:G:132:GLY:HA2	1.94	0.50
1:D:110:THR:HG23	1:D:113:GLU:OE1	2.12	0.50
1:J:46:VAL:O	1:J:50:MET:HB2	2.12	0.49
1:H:72:TYR:OH	1:H:154[B]:SER:OG	2.25	0.49
1:K:114:GLN:NE2	1:K:117[B]:ARG:NH2	2.58	0.49
1:B:58:TRP:CH2	1:J:56:MET:HE3	2.47	0.49
1:E:60:PRO:O	1:E:63:ASP:HB2	2.12	0.49
1:B:62:MET:O	1:B:66[B]:MET:HG3	2.12	0.49
1:L:114:GLN:HA	1:L:114:GLN:NE2	2.24	0.49
1:E:171:LYS:HE3	6:E:2038:HOH:O	2.11	0.49
1:H:68:GLU:OE2	1:H:72:TYR:OH	2.30	0.49
1:D:22:LEU:HD13	1:D:83:LEU:HD22	1.95	0.48
1:I:28:VAL:HG21	1:I:132:GLY:HA2	1.95	0.48
1:I:22:LEU:HD23	1:I:83:LEU:HD22	1.96	0.48
1:B:96:GLU:HG2	6:B:2044:HOH:O	2.14	0.48
1:A:60:PRO:O	1:A:63:ASP:HB2	2.14	0.48
1:I:47:HIS:CE1	1:I:59:HIS:CE1	3.02	0.48
1:D:152:LYS:HE3	6:D:2077:HOH:O	2.14	0.48
1:B:57:ILE:HD12	3:B:1173:EPE:O3S	2.14	0.47
1:I:123[B]:ARG:NH1	6:I:2045:HOH:O	2.36	0.47
1:G:130:GLN:NE2	1:G:152:LYS:HE2	2.29	0.47
1:B:168:GLN:NE2	1:B:171:LYS:NZ	2.62	0.46
1:I:24:ASP:HB2	1:I:139:GLU:OE2	2.15	0.46
1:G:56:MET:HE3	1:I:58:TRP:CH2	2.51	0.46
1:H:142:SER:OG	1:J:149:ASN:ND2	2.48	0.46
1:H:57:ILE:HG23	1:H:58:TRP:CD1	2.51	0.46
1:H:78[B]:GLU:OE2	1:J:157:LYS:HE3	2.17	0.45
1:L:46:VAL:HG12	1:L:50:MET:HE3	1.98	0.45
1:L:77[A]:SER:O	1:L:80:LEU:HB3	2.16	0.45
1:J:57:ILE:HG23	1:J:58:TRP:CD1	2.52	0.45
1:L:78[A]:GLU:HA	1:L:81:ILE:HD12	1.98	0.45
1:C:135:VAL:O	1:C:139:GLU:HG3	2.17	0.45
1:K:130:GLN:HE22	1:K:152:LYS:NZ	2.16	0.44
1:C:78:GLU:HG2	1:H:160:TRP:CH2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:GLU:OE2	1:E:72:TYR:OH	2.36	0.44
1:K:47:HIS:CE1	1:K:59:HIS:CE1	3.06	0.44
1:B:28:VAL:HG11	1:B:132:GLY:HA2	2.00	0.44
1:L:46:VAL:O	1:L:50:MET:HB2	2.17	0.44
1:K:53:ARG:HB3	3:K:1173:EPE:H21	1.99	0.43
1:B:99:GLN:HG3	1:B:124:TYR:OH	2.17	0.43
1:E:47:HIS:CE1	1:E:59:HIS:CE1	3.05	0.43
1:F:32:ALA:HA	1:F:128:LEU:HD21	2.00	0.43
1:I:44:HIS:CD2	6:I:2003:HOH:O	2.70	0.43
1:K:117[B]:ARG:HG3	1:K:117[B]:ARG:HH21	1.83	0.43
1:B:168:GLN:NE2	1:B:171:LYS:HZ1	2.12	0.43
1:C:46:VAL:O	1:C:50:MET:HB2	2.19	0.43
1:K:114:GLN:HA	1:K:114:GLN:NE2	2.27	0.43
1:B:47:HIS:CE1	1:B:59:HIS:CE1	3.07	0.43
1:A:50:MET:HG3	1:A:111:ILE:HD13	1.99	0.43
1:C:32:ALA:HA	1:C:128:LEU:HD21	2.00	0.43
1:D:58:TRP:HH2	1:I:56:MET:HE3	1.83	0.42
1:G:40:HIS:CE1	1:G:70:ASP:OD1	2.72	0.42
1:A:48:TRP:HB3	1:C:81:ILE:HD11	2.02	0.42
1:J:61:LYS:HA	1:J:61:LYS:HD3	1.90	0.42
1:L:65:TYR:O	1:L:69:ILE:HG12	2.20	0.42
1:G:142:SER:OG	1:L:149:ASN:ND2	2.53	0.42
1:J:47:HIS:CE1	1:J:59:HIS:CE1	3.07	0.42
1:I:50:MET:HG3	1:I:111:ILE:HD13	2.02	0.42
1:I:57:ILE:HD12	1:I:58:TRP:CD1	2.54	0.42
1:I:115:LEU:HB2	1:I:166:LEU:HD21	2.02	0.42
1:L:46:VAL:HG13	1:L:114:GLN:HB3	2.01	0.42
1:G:46:VAL:O	1:G:50:MET:HB2	2.19	0.42
1:A:56:MET:HE1	1:H:161:MET:HB3	2.02	0.42
1:F:143:VAL:HG23	1:K:152:LYS:HE2	2.02	0.41
1:L:114:GLN:HE21	1:L:114:GLN:CA	2.21	0.41
1:D:46:VAL:O	1:D:50:MET:HB2	2.19	0.41
1:D:32:ALA:HA	1:D:128:LEU:HD21	2.01	0.41
1:D:161:MET:HB3	1:I:56:MET:HE1	2.02	0.41
1:I:29:LEU:HD21	1:I:144:THR:HG23	2.02	0.41
1:I:57:ILE:CD1	1:I:58:TRP:CD1	3.04	0.41
1:A:38:VAL:O	1:A:42:ILE:HG13	2.21	0.41
1:F:24:ASP:HB3	1:F:135:VAL:HG13	2.01	0.41
1:J:22:LEU:HD12	1:J:83:LEU:HD22	2.03	0.41
1:K:26:LYS:HE2	1:K:83:LEU:O	2.21	0.41
1:I:32:ALA:HA	1:I:128:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:VAL:O	1:H:50:MET:HB2	2.21	0.40
1:K:72:TYR:OH	1:K:154[B]:SER:OG	2.38	0.40
1:D:157:LYS:HG2	6:D:2087:HOH:O	2.21	0.40
1:I:130:GLN:HE21	1:I:152:LYS:HE3	1.85	0.40
1:E:114:GLN:O	1:E:118:VAL:HG23	2.21	0.40
3:G:1173:EPE:H101	3:G:1173:EPE:H22	1.85	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	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	B	152/165 (92%)	151 (99%)	1 (1%)	0	100	100
1	C	148/165 (90%)	147 (99%)	1 (1%)	0	100	100
1	D	155/165 (94%)	154 (99%)	1 (1%)	0	100	100
1	E	152/165 (92%)	151 (99%)	1 (1%)	0	100	100
1	F	152/165 (92%)	151 (99%)	1 (1%)	0	100	100
1	G	151/165 (92%)	149 (99%)	2 (1%)	0	100	100
1	H	151/165 (92%)	149 (99%)	2 (1%)	0	100	100
1	I	152/165 (92%)	150 (99%)	2 (1%)	0	100	100
1	J	152/165 (92%)	151 (99%)	1 (1%)	0	100	100
1	K	156/165 (94%)	155 (99%)	1 (1%)	0	100	100
1	L	156/165 (94%)	154 (99%)	2 (1%)	0	100	100
All	All	1827/1980 (92%)	1811 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	130/141 (92%)	127 (98%)	3 (2%)	44	51
1	B	131/141 (93%)	126 (96%)	5 (4%)	29	32
1	C	127/141 (90%)	121 (95%)	6 (5%)	23	24
1	D	135/141 (96%)	133 (98%)	2 (2%)	57	65
1	E	130/141 (92%)	127 (98%)	3 (2%)	44	51
1	F	132/141 (94%)	131 (99%)	1 (1%)	73	81
1	G	132/141 (94%)	130 (98%)	2 (2%)	57	65
1	H	130/141 (92%)	124 (95%)	6 (5%)	24	25
1	I	129/141 (92%)	121 (94%)	8 (6%)	16	14
1	J	130/141 (92%)	126 (97%)	4 (3%)	35	39
1	K	135/141 (96%)	130 (96%)	5 (4%)	30	33
1	L	135/141 (96%)	128 (95%)	7 (5%)	21	20
All	All	1576/1692 (93%)	1524 (97%)	52 (3%)	33	37

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

Mol	Chain	Res	Type
1	A	44	HIS
1	A	131	LYS
1	A	146	ASP
1	B	44	HIS
1	B	69	ILE
1	B	73	LEU
1	B	111	ILE
1	B	155	ILE
1	C	44	HIS
1	C	73	LEU
1	C	95	SER
1	C	99	GLN
1	C	146	ASP
1	C	149	ASN

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Mol	Chain	Res	Type
1	D	44	HIS
1	D	69	ILE
1	E	44	HIS
1	E	74	ASP
1	E	146	ASP
1	F	44	HIS
1	G	44	HIS
1	G	138	GLU
1	H	44	HIS
1	H	92	LYS
1	H	99	GLN
1	H	101	LYS
1	H	112	GLU
1	H	135	VAL
1	I	44	HIS
1	I	57	ILE
1	I	69	ILE
1	I	70	ASP
1	I	99	GLN
1	I	101	LYS
1	I	114	GLN
1	I	117	ARG
1	J	44	HIS
1	J	114	GLN
1	J	117	ARG
1	J	149	ASN
1	K	44	HIS
1	K	114	GLN
1	K	117[A]	ARG
1	K	117[B]	ARG
1	K	135	VAL
1	L	22	LEU
1	L	44	HIS
1	L	95[A]	SER
1	L	95[B]	SER
1	L	111	ILE
1	L	114	GLN
1	L	131	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	45	GLN
1	A	130	GLN
1	A	149	ASN
1	A	168	GLN
1	B	44	HIS
1	B	130	GLN
1	B	149	ASN
1	B	163	GLN
1	B	168	GLN
1	C	31	GLN
1	C	40	HIS
1	C	45	GLN
1	C	99	GLN
1	C	130	GLN
1	C	149	ASN
1	D	130	GLN
1	D	149	ASN
1	E	130	GLN
1	E	149	ASN
1	F	130	GLN
1	F	149	ASN
1	F	163	GLN
1	G	40	HIS
1	G	130	GLN
1	G	149	ASN
1	H	31	GLN
1	H	44	HIS
1	H	130	GLN
1	H	149	ASN
1	H	163	GLN
1	I	44	HIS
1	I	114	GLN
1	I	130	GLN
1	I	149	ASN
1	I	163	GLN
1	J	45	GLN
1	J	114	GLN
1	J	130	GLN
1	J	149	ASN
1	K	44	HIS
1	K	108	ASN
1	K	114	GLN

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Mol	Chain	Res	Type
1	K	130	GLN
1	K	149	ASN
1	L	45	GLN
1	L	99	GLN
1	L	114	GLN
1	L	130	GLN
1	L	149	ASN
1	L	163	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 25 are monoatomic - leaving 4 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	EPE	G	1173	-	15,15,15	0.72	0	19,20,20	1.74	4 (21%)
3	EPE	B	1173	-	15,15,15	0.90	1 (6%)	19,20,20	2.04	6 (31%)
3	EPE	K	1173	-	15,15,15	1.03	1 (6%)	19,20,20	1.73	5 (26%)
3	EPE	L	1173	-	15,15,15	0.82	1 (6%)	19,20,20	2.02	6 (31%)

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	EPE	G	1173	-	-	6/9/19/19	0/1/1/1
3	EPE	B	1173	-	-	6/9/19/19	0/1/1/1
3	EPE	K	1173	-	-	3/9/19/19	0/1/1/1
3	EPE	L	1173	-	-	4/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1173	EPE	C10-S	3.38	1.82	1.77
3	L	1173	EPE	C10-S	2.71	1.81	1.77
3	B	1173	EPE	C10-S	2.58	1.81	1.77

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1173	EPE	O1S-S-C10	5.11	114.45	106.73
3	L	1173	EPE	C5-N4-C3	4.44	118.40	108.84
3	L	1173	EPE	O1S-S-C10	4.24	113.14	106.73
3	K	1173	EPE	C5-N4-C3	4.20	117.88	108.84
3	B	1173	EPE	C5-N4-C3	3.96	117.37	108.84
3	G	1173	EPE	C5-N4-C3	3.86	117.15	108.84
3	G	1173	EPE	O2S-S-C10	3.81	112.48	106.73
3	L	1173	EPE	C7-N4-C3	3.54	120.67	111.24
3	B	1173	EPE	C6-N1-C2	2.99	115.28	108.84
3	K	1173	EPE	O3S-S-C10	2.97	111.82	106.00
3	L	1173	EPE	O2S-S-C10	-2.93	102.30	106.73
3	G	1173	EPE	C6-N1-C2	2.92	115.14	108.84
3	K	1173	EPE	O1S-S-C10	2.77	110.91	106.73
3	L	1173	EPE	C7-N4-C5	2.65	118.30	111.24
3	B	1173	EPE	C7-N4-C3	2.56	118.07	111.24
3	G	1173	EPE	C7-N4-C5	2.56	118.07	111.24
3	K	1173	EPE	O3S-S-O2S	-2.33	105.58	111.40
3	K	1173	EPE	C7-N4-C5	2.32	117.41	111.24
3	B	1173	EPE	C10-C9-N1	-2.16	104.19	112.36
3	B	1173	EPE	C7-N4-C5	2.15	116.96	111.24
3	L	1173	EPE	O3S-S-C10	2.03	109.98	106.00

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1173	EPE	C10-C9-N1-C2
3	G	1173	EPE	C10-C9-N1-C2
3	K	1173	EPE	C10-C9-N1-C2
3	L	1173	EPE	C9-C10-S-O2S
3	L	1173	EPE	N4-C7-C8-O8
3	B	1173	EPE	C9-C10-S-O3S
3	G	1173	EPE	C9-C10-S-O3S
3	L	1173	EPE	C9-C10-S-O3S
3	B	1173	EPE	C8-C7-N4-C5
3	B	1173	EPE	C10-C9-N1-C6
3	K	1173	EPE	C10-C9-N1-C6
3	K	1173	EPE	C8-C7-N4-C3
3	B	1173	EPE	C9-C10-S-O1S
3	B	1173	EPE	C9-C10-S-O2S
3	G	1173	EPE	C9-C10-S-O1S
3	G	1173	EPE	C9-C10-S-O2S
3	L	1173	EPE	C9-C10-S-O1S
3	G	1173	EPE	C8-C7-N4-C3
3	G	1173	EPE	N4-C7-C8-O8

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1173	EPE	1	0
3	B	1173	EPE	1	0
3	K	1173	EPE	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 ⓘ

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	150/165 (90%)	-0.03	2 (1%) 75 77	19, 45, 61, 67	2 (1%)
1	B	151/165 (91%)	-0.17	1 (0%) 84 86	17, 36, 52, 73	3 (1%)
1	C	150/165 (90%)	0.04	1 (0%) 84 86	40, 47, 63, 79	0
1	D	152/165 (92%)	-0.21	0 100 100	14, 35, 49, 67	5 (3%)
1	E	151/165 (91%)	0.11	1 (0%) 84 86	20, 49, 65, 81	3 (1%)
1	F	151/165 (91%)	-0.19	2 (1%) 75 77	17, 36, 53, 60	3 (1%)
1	G	149/165 (90%)	0.04	0 100 100	18, 46, 63, 72	4 (2%)
1	H	151/165 (91%)	0.03	0 100 100	17, 44, 64, 76	2 (1%)
1	I	151/165 (91%)	0.01	1 (0%) 84 86	22, 44, 63, 80	3 (1%)
1	J	151/165 (91%)	-0.06	1 (0%) 84 86	20, 41, 58, 68	3 (1%)
1	K	152/165 (92%)	-0.19	0 100 100	15, 39, 51, 59	6 (3%)
1	L	152/165 (92%)	-0.06	1 (0%) 84 86	15, 41, 55, 65	6 (3%)
All	All	1811/1980 (91%)	-0.06	10 (0%) 85 87	14, 43, 62, 81	40 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	21	SER	4.7
1	E	23	ALA	4.0
1	I	138	GLU	2.9
1	B	23	ALA	2.3
1	A	140	GLY	2.3
1	J	22	LEU	2.2
1	C	23	ALA	2.2
1	A	23	ALA	2.1
1	F	23	ALA	2.1
1	F	22	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 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	CA	F	1175	1/1	0.90	0.16	29,29,29,29	0
4	CA	B	1175	1/1	0.91	0.25	28,28,28,28	0
4	CA	I	1175	1/1	0.91	0.20	38,38,38,38	0
4	CA	J	1175	1/1	0.91	0.16	36,36,36,36	0
2	NI	G	1174	1/1	0.93	0.14	27,27,27,27	0
5	CL	D	1174	1/1	0.93	0.24	26,26,26,26	0
3	EPE	K	1173	15/15	0.94	0.10	19,28,35,38	0
3	EPE	L	1173	15/15	0.94	0.11	20,38,47,48	0
3	EPE	G	1173	15/15	0.94	0.10	20,25,32,35	0
4	CA	D	1175	1/1	0.94	0.14	38,38,38,38	0
5	CL	I	1174	1/1	0.94	0.22	22,22,22,22	0
5	CL	J	1174	1/1	0.94	0.25	19,19,19,19	0
4	CA	F	1174	1/1	0.95	0.19	9,9,9,9	0
5	CL	E	1174	1/1	0.95	0.14	36,36,36,36	0
4	CA	K	1175	1/1	0.95	0.06	48,48,48,48	0
5	CL	B	1176	1/1	0.95	0.29	16,16,16,16	0
2	NI	C	1173	1/1	0.96	0.19	22,22,22,22	0
5	CL	G	1175	1/1	0.96	0.23	23,23,23,23	0
2	NI	I	1173	1/1	0.96	0.26	12,12,12,12	0
3	EPE	B	1173	15/15	0.96	0.10	15,26,32,33	0
2	NI	E	1173	1/1	0.98	0.19	19,19,19,19	0
2	NI	J	1173	1/1	0.98	0.27	10,10,10,10	0
2	NI	L	1174	1/1	0.98	0.15	17,17,17,17	0
2	NI	A	1173	1/1	0.98	0.23	12,12,12,12	0
2	NI	H	1173	1/1	0.99	0.15	16,16,16,16	0
2	NI	F	1173	1/1	0.99	0.26	5,5,5,5	0
2	NI	D	1173	1/1	0.99	0.18	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	B	1174	1/1	1.00	0.23	4,4,4,4	0
2	NI	K	1174	1/1	1.00	0.15	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.