



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:48 PM UTC

PDB ID : 2XKQ / pdb_00002xkq
Title : Crystal structure of Streptococcus suis Dpr with manganese
Authors : Haikarainen, T.; Thanassoulas, A.; Stavros, P.; Nounesis, G.; Haataja, S.;
Papageorgiou, A.C.
Deposited on : 2010-07-12
Resolution : 2.40 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

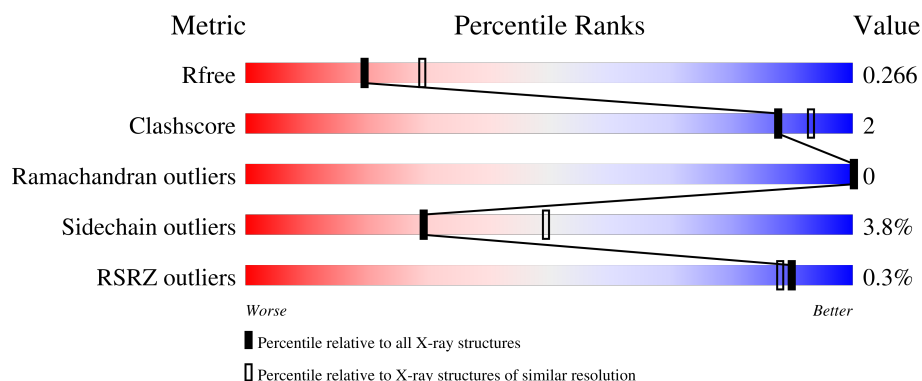
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	
1	B	165	
1	C	165	
1	D	165	
1	E	165	

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Mol	Chain	Length	Quality of chain
1	F	165	90% .. 8%
1	G	165	% 81% 10% 8%
1	H	165	83% 8% • 8%
1	I	165	% 85% 5% • 9%
1	J	165	% 87% 5% 8%
1	K	165	82% 10% 8%
1	L	165	81% 9% • 8%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15132 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	151	Total	C	N	O	S	0	0	0
			1209	771	199	233	6			
1	B	151	Total	C	N	O	S	0	1	0
			1211	772	199	234	6			
1	C	149	Total	C	N	O	S	0	1	0
			1198	763	197	232	6			
1	D	152	Total	C	N	O	S	0	1	0
			1217	775	200	236	6			
1	E	151	Total	C	N	O	S	0	1	0
			1207	769	198	234	6			
1	F	151	Total	C	N	O	S	0	0	0
			1209	771	199	233	6			
1	G	151	Total	C	N	O	S	0	0	0
			1209	771	199	233	6			
1	H	151	Total	C	N	O	S	0	1	0
			1208	769	199	234	6			
1	I	150	Total	C	N	O	S	0	2	0
			1205	767	198	234	6			
1	J	152	Total	C	N	O	S	0	1	0
			1216	774	199	237	6			
1	K	152	Total	C	N	O	S	0	2	0
			1219	776	200	237	6			
1	L	151	Total	C	N	O	S	0	2	0
			1213	773	199	235	6			

- Molecule 2 is MANGANESE (III) ION (CCD ID: MN3) (formula: Mn).

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

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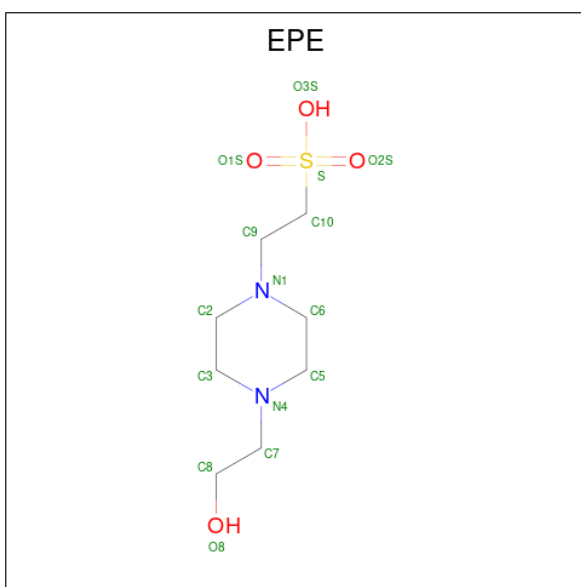
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	E	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0
2	G	1	Total 1	Mn 1	0	0
2	H	1	Total 1	Mn 1	0	0
2	I	1	Total 1	Mn 1	0	0
2	J	1	Total 1	Mn 1	0	0
2	K	1	Total 1	Mn 1	0	0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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0
3	I	1	Total 1	Cl 1	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	D	1	Total	Ca	0	0
			1	1		
5	F	2	Total	Ca	0	0
			2	2		
5	G	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total	O	0	0
			34	34		

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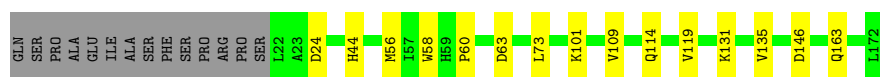
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	59	Total 59	O 59	0	0
6	C	29	Total 29	O 29	0	0
6	D	58	Total 58	O 58	0	0
6	E	31	Total 31	O 31	0	0
6	F	60	Total 60	O 60	0	0
6	G	30	Total 30	O 30	0	0
6	H	42	Total 42	O 42	0	0
6	I	43	Total 43	O 43	0	0
6	J	49	Total 49	O 49	0	0
6	K	54	Total 54	O 54	0	0
6	L	40	Total 40	O 40	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.

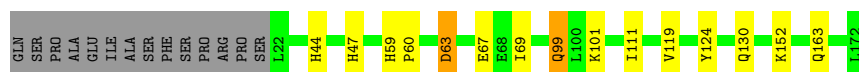
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain A: 



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain B: 



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain C: 



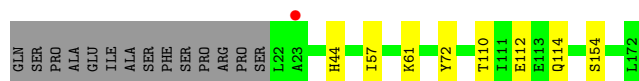
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain D: 



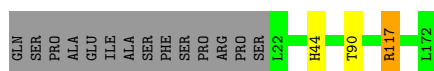
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain E: 

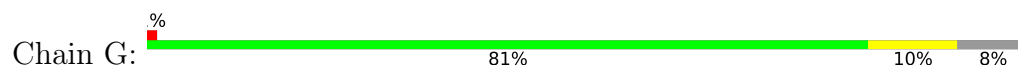


• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

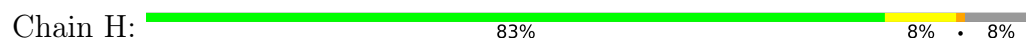
Chain F: 



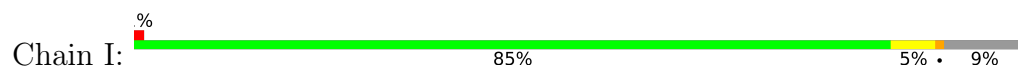
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



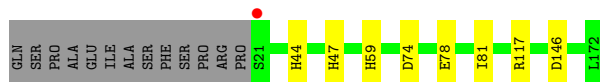
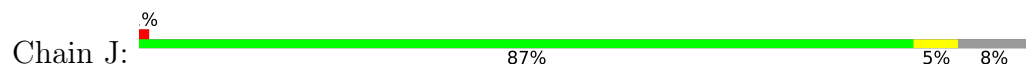
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



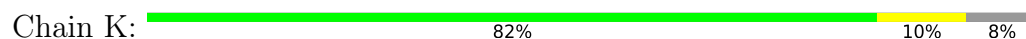
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



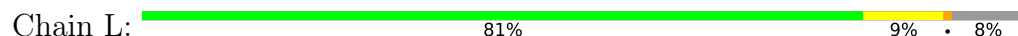
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.22Å 139.47Å 143.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.40 49.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.00-2.40) 99.8 (49.00-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.4.0078	Depositor
R, R_{free}	0.183 , 0.245 0.208 , 0.266	Depositor DCC
R_{free} test set	4190 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15132	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.52% 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, MN3, CA, 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	0.85	0/1234	0.96	0/1666
1	B	0.96	0/1240	1.00	0/1674
1	C	0.78	0/1227	0.93	0/1656
1	D	0.92	0/1246	0.98	0/1682
1	E	0.81	0/1236	0.94	1/1670 (0.1%)
1	F	0.94	0/1234	0.98	0/1666
1	G	0.82	0/1234	0.99	0/1666
1	H	0.86	0/1237	1.00	2/1670 (0.1%)
1	I	0.89	0/1238	0.97	0/1671
1	J	0.86	0/1245	0.95	0/1682
1	K	0.87	1/1252 (0.1%)	0.99	0/1690
1	L	0.86	1/1246 (0.1%)	0.98	0/1682
All	All	0.87	2/14869 (0.0%)	0.97	3/20075 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	57	ILE	CA-CB	6.05	1.61	1.54
1	K	150	VAL	CA-CB	5.02	1.60	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	57	ILE	N-CA-C	5.03	115.70	110.82
1	H	59	HIS	CA-C-N	-5.01	113.88	119.19
1	H	59	HIS	C-N-CA	-5.01	113.88	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	1209	0	1174	7	0
1	B	1211	0	1175	6	0
1	C	1198	0	1159	5	0
1	D	1217	0	1180	4	0
1	E	1207	0	1164	4	0
1	F	1209	0	1174	5	0
1	G	1209	0	1174	7	0
1	H	1208	0	1166	7	0
1	I	1205	0	1165	4	0
1	J	1216	0	1170	3	0
1	K	1219	0	1181	6	0
1	L	1213	0	1176	8	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	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
4	B	15	0	17	0	0
4	D	15	0	17	1	0
4	E	15	0	17	0	0
4	K	15	0	17	0	0
5	B	2	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
6	A	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	59	0	0	1	0
6	C	29	0	0	1	0
6	D	58	0	0	1	0
6	E	31	0	0	0	0
6	F	60	0	0	0	0
6	G	30	0	0	0	0
6	H	42	0	0	2	0
6	I	43	0	0	0	0
6	J	49	0	0	0	0
6	K	54	0	0	1	0
6	L	40	0	0	1	0
All	All	15132	0	14126	57	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 2.

All (57) 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:J:74:ASP:O	1:J:78:GLU:HG3	1.77	0.84
1:F:117:ARG:HH11	1:F:117:ARG:HG3	1.46	0.80
1:A:24:ASP:HB3	1:A:135:VAL:HG11	1.66	0.78
1:K:75:GLU:HG3	6:K:2021:HOH:O	1.93	0.69
1:G:78:GLU:OE1	1:L:157:LYS:NZ	2.33	0.61
1:C:24:ASP:HB2	1:C:139:GLU:OE2	2.01	0.61
1:G:59:HIS:HB3	1:G:60:PRO:HD3	1.85	0.57
1:B:130:GLN:NE2	1:B:152:LYS:HE2	2.20	0.57
1:L:46:VAL:HG13	1:L:114:GLN:HB3	1.88	0.56
1:C:47:HIS:CE1	1:C:59:HIS:CE1	2.95	0.55
1:K:59:HIS:HB3	1:K:60:PRO:HD3	1.89	0.55
1:F:90:THR:HG22	1:H:102:GLU:HB3	1.91	0.52
1:G:119:VAL:HG21	1:G:163:GLN:HE21	1.74	0.52
1:H:119:VAL:HG21	1:H:163:GLN:HE21	1.75	0.51
1:B:67:GLU:HB2	6:B:2019:HOH:O	2.10	0.51
1:A:58:TRP:CH2	1:K:56:MET:HE3	2.46	0.51
1:G:56:MET:HE3	1:I:58:TRP:CH2	2.46	0.51
1:A:109:VAL:HG12	1:A:114:GLN:HG2	1.91	0.50
1:C:56:MET:HE3	1:E:61:LYS:HE3	1.94	0.48
1:B:99:GLN:HG3	1:B:124:TYR:OH	2.13	0.48
1:J:47:HIS:CE1	1:J:59:HIS:CE1	3.03	0.47
1:H:44:HIS:HD2	6:H:2004:HOH:O	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:138:GLU:OE2	1:L:138:GLU:HA	2.15	0.47
1:D:58:TRP:CH2	1:I:56:MET:HE3	2.50	0.47
1:F:117:ARG:HH11	1:F:117:ARG:CG	2.20	0.47
1:C:60:PRO:O	1:C:63:ASP:HB2	2.15	0.46
1:K:78:GLU:HA	1:K:81:ILE:HD12	1.98	0.45
1:C:44:HIS:HD2	6:C:2002:HOH:O	2.00	0.45
1:A:60:PRO:O	1:A:63:ASP:HB2	2.16	0.45
1:B:47:HIS:CE1	1:B:59:HIS:CE1	3.05	0.45
1:G:155:ILE:HD13	1:G:155:ILE:HA	1.88	0.44
1:E:72:TYR:OH	1:E:154[B]:SER:OG	2.28	0.44
1:F:90:THR:HB	6:H:2032:HOH:O	2.16	0.44
1:A:119:VAL:HG21	1:A:163:GLN:HE21	1.83	0.44
1:E:72:TYR:HH	1:E:154[B]:SER:HG	1.53	0.43
1:B:119:VAL:HG21	1:B:163:GLN:HE21	1.82	0.43
1:H:152:LYS:O	1:H:156:GLU:HG3	2.18	0.43
1:E:110:THR:O	1:E:114:GLN:HG2	2.19	0.43
1:I:119:VAL:HG21	1:I:163:GLN:HE21	1.83	0.43
1:D:163:GLN:NE2	6:D:2054:HOH:O	2.38	0.43
1:F:117:ARG:HG3	1:F:117:ARG:NH1	2.26	0.43
1:L:130:GLN:NE2	1:L:152:LYS:HE2	2.34	0.43
1:A:58:TRP:HH2	1:K:56:MET:HE3	1.83	0.42
1:H:56:MET:HE1	1:K:161:MET:HB3	2.01	0.42
1:L:46:VAL:HG12	1:L:50:MET:HE3	2.02	0.42
1:J:78:GLU:HA	1:J:81:ILE:HD12	2.02	0.42
1:I:60:PRO:O	1:I:63:ASP:HB2	2.20	0.42
1:H:68:GLU:OE2	1:H:154[B]:SER:OG	2.34	0.41
1:L:112:GLU:HG3	6:L:2029:HOH:O	2.20	0.41
1:G:63:ASP:HA	1:G:66:MET:HE3	2.01	0.41
1:B:60:PRO:O	1:B:63:ASP:HB2	2.20	0.41
1:L:47:HIS:CE1	1:L:59:HIS:CE1	3.09	0.41
1:G:76:MET:HE1	1:G:129:PHE:CE2	2.56	0.41
1:L:149:ASN:HD22	1:L:149:ASN:HA	1.77	0.41
1:D:57:ILE:HD12	4:D:1173:EPE:O1S	2.21	0.41
1:A:56:MET:HE3	1:H:58:TRP:CH2	2.57	0.40
1:D:160:TRP:CD1	1:D:160:TRP:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	149/165 (90%)	147 (99%)	2 (1%)	0	100	100
1	B	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	C	148/165 (90%)	146 (99%)	2 (1%)	0	100	100
1	D	151/165 (92%)	150 (99%)	1 (1%)	0	100	100
1	E	150/165 (91%)	148 (99%)	2 (1%)	0	100	100
1	F	149/165 (90%)	148 (99%)	1 (1%)	0	100	100
1	G	149/165 (90%)	147 (99%)	2 (1%)	0	100	100
1	H	150/165 (91%)	148 (99%)	2 (1%)	0	100	100
1	I	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	J	151/165 (92%)	150 (99%)	1 (1%)	0	100	100
1	K	152/165 (92%)	151 (99%)	1 (1%)	0	100	100
1	L	151/165 (92%)	149 (99%)	2 (1%)	0	100	100
All	All	1800/1980 (91%)	1782 (99%)	18 (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	129/141 (92%)	124 (96%)	5 (4%)	28	48
1	B	130/141 (92%)	124 (95%)	6 (5%)	24	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	129/141 (92%)	122 (95%)	7 (5%)	20	35
1	D	131/141 (93%)	126 (96%)	5 (4%)	29	49
1	E	129/141 (92%)	127 (98%)	2 (2%)	55	76
1	F	129/141 (92%)	127 (98%)	2 (2%)	55	76
1	G	129/141 (92%)	123 (95%)	6 (5%)	23	41
1	H	129/141 (92%)	125 (97%)	4 (3%)	35	57
1	I	130/141 (92%)	126 (97%)	4 (3%)	35	57
1	J	130/141 (92%)	127 (98%)	3 (2%)	44	66
1	K	132/141 (94%)	123 (93%)	9 (7%)	14	25
1	L	131/141 (93%)	124 (95%)	7 (5%)	20	36
All	All	1558/1692 (92%)	1498 (96%)	60 (4%)	29	48

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	73	LEU
1	A	101	LYS
1	A	131	LYS
1	A	146	ASP
1	B	44	HIS
1	B	63	ASP
1	B	69	ILE
1	B	99	GLN
1	B	101	LYS
1	B	111	ILE
1	C	24	ASP
1	C	44	HIS
1	C	56	MET
1	C	57	ILE
1	C	117	ARG
1	C	120	GLU
1	C	149	ASN
1	D	44	HIS
1	D	95	SER
1	D	99	GLN
1	D	101	LYS
1	D	146	ASP

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Mol	Chain	Res	Type
1	E	44	HIS
1	E	112	GLU
1	F	44	HIS
1	F	117	ARG
1	G	44	HIS
1	G	69	ILE
1	G	101	LYS
1	G	146	ASP
1	G	149	ASN
1	G	154	SER
1	H	44	HIS
1	H	95	SER
1	H	101	LYS
1	H	138	GLU
1	I	44	HIS
1	I	63	ASP
1	I	117	ARG
1	I	135	VAL
1	J	44	HIS
1	J	117	ARG
1	J	146	ASP
1	K	44	HIS
1	K	67	GLU
1	K	95[A]	SER
1	K	95[B]	SER
1	K	101	LYS
1	K	111	ILE
1	K	112	GLU
1	K	135	VAL
1	K	149	ASN
1	L	22	LEU
1	L	44	HIS
1	L	111	ILE
1	L	131	LYS
1	L	135	VAL
1	L	138	GLU
1	L	149	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS

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

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Mol	Chain	Res	Type
1	K	149	ASN
1	K	163	GLN
1	L	44	HIS
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 26 ligands modelled in this entry, 22 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$
4	EPE	D	1173	-	15,15,15	0.90	1 (6%)	19,20,20	1.97	8 (42%)
4	EPE	E	1173	-	15,15,15	0.98	1 (6%)	19,20,20	1.90	4 (21%)
4	EPE	B	1173	-	15,15,15	0.81	1 (6%)	19,20,20	2.01	5 (26%)
4	EPE	K	1173	-	15,15,15	0.93	1 (6%)	19,20,20	2.09	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
4	EPE	D	1173	-	-	5/9/19/19	0/1/1/1
4	EPE	E	1173	-	-	7/9/19/19	0/1/1/1
4	EPE	B	1173	-	-	6/9/19/19	0/1/1/1
4	EPE	K	1173	-	-	3/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1173	EPE	C10-S	3.16	1.82	1.77
4	E	1173	EPE	C10-S	3.13	1.82	1.77
4	D	1173	EPE	C10-S	2.77	1.81	1.77
4	B	1173	EPE	C10-S	2.50	1.81	1.77

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1173	EPE	C5-N4-C3	5.54	120.78	108.84
4	B	1173	EPE	O3S-S-C10	4.96	115.71	106.00
4	E	1173	EPE	O2S-S-C10	4.64	113.74	106.73
4	B	1173	EPE	C5-N4-C3	4.44	118.40	108.84
4	E	1173	EPE	C5-N4-C3	4.43	118.38	108.84
4	D	1173	EPE	C6-N1-C2	3.88	117.20	108.84
4	D	1173	EPE	O3S-S-C10	3.73	113.30	106.00
4	K	1173	EPE	C7-N4-C3	3.17	119.68	111.24
4	E	1173	EPE	C6-N1-C2	3.15	115.62	108.84
4	K	1173	EPE	C7-N4-C5	3.03	119.31	111.24
4	B	1173	EPE	C7-N4-C3	2.99	119.20	111.24
4	K	1173	EPE	O2S-S-C10	2.91	111.13	106.73
4	K	1173	EPE	O1S-S-C10	2.80	110.95	106.73
4	D	1173	EPE	C7-N4-C5	2.60	118.18	111.24
4	D	1173	EPE	C7-N4-C3	2.60	118.17	111.24
4	D	1173	EPE	C5-C6-N1	2.60	115.89	110.65
4	D	1173	EPE	C5-N4-C3	2.58	114.39	108.84
4	B	1173	EPE	C7-N4-C5	2.40	117.65	111.24
4	D	1173	EPE	O2S-S-C10	2.35	110.28	106.73
4	E	1173	EPE	C7-N4-C3	2.26	117.26	111.24
4	D	1173	EPE	C3-C2-N1	2.25	115.18	110.65
4	K	1173	EPE	C9-N1-C6	-2.07	105.71	111.24
4	B	1173	EPE	C10-C9-N1	-2.05	104.62	112.36

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	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	151/165 (91%)	-0.17	0	100 100	31, 41, 56, 66	0
1	B	151/165 (91%)	-0.35	0	100 100	22, 34, 48, 68	1 (0%)
1	C	149/165 (90%)	-0.26	0	100 100	27, 42, 58, 73	1 (0%)
1	D	152/165 (92%)	-0.40	1 (0%)	84 81	21, 33, 48, 60	1 (0%)
1	E	151/165 (91%)	-0.04	1 (0%)	84 81	29, 45, 61, 77	1 (0%)
1	F	151/165 (91%)	-0.39	0	100 100	24, 33, 49, 56	0
1	G	151/165 (91%)	-0.10	2 (1%)	75 71	33, 43, 60, 76	0
1	H	151/165 (91%)	-0.15	0	100 100	28, 40, 57, 70	1 (0%)
1	I	150/165 (90%)	-0.18	1 (0%)	84 81	27, 40, 59, 79	2 (1%)
1	J	152/165 (92%)	-0.33	1 (0%)	84 81	22, 38, 55, 76	1 (0%)
1	K	152/165 (92%)	-0.36	0	100 100	23, 36, 48, 56	2 (1%)
1	L	151/165 (91%)	-0.31	0	100 100	25, 38, 51, 63	2 (1%)
All	All	1812/1980 (91%)	-0.25	6 (0%)	90 88	21, 39, 57, 79	12 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	23	ALA	4.5
1	G	23	ALA	3.7
1	G	22	LEU	2.7
1	I	138	GLU	2.3
1	D	21	SER	2.0
1	J	21	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
5	CA	D	1175	1/1	0.82	0.18	29,29,29,29	0
5	CA	B	1176	1/1	0.86	0.09	58,58,58,58	0
3	CL	C	1174	1/1	0.88	0.11	33,33,33,33	0
3	CL	I	1174	1/1	0.91	0.22	25,25,25,25	0
5	CA	B	1175	1/1	0.91	0.10	42,42,42,42	0
5	CA	G	1174	1/1	0.91	0.12	26,26,26,26	0
4	EPE	D	1173	15/15	0.92	0.13	17,23,28,28	0
4	EPE	E	1173	15/15	0.92	0.13	17,27,33,33	0
4	EPE	K	1173	15/15	0.93	0.12	18,25,33,33	0
2	MN3	G	1173	1/1	0.94	0.09	34,34,34,34	0
2	MN3	B	1174	1/1	0.95	0.18	14,14,14,14	0
4	EPE	B	1173	15/15	0.95	0.12	16,26,34,35	0
5	CA	F	1175	1/1	0.95	0.09	33,33,33,33	0
2	MN3	F	1173	1/1	0.95	0.19	13,13,13,13	0
2	MN3	D	1174	1/1	0.96	0.13	20,20,20,20	0
2	MN3	K	1174	1/1	0.96	0.12	21,21,21,21	0
2	MN3	L	1173	1/1	0.96	0.09	23,23,23,23	0
2	MN3	A	1173	1/1	0.96	0.12	20,20,20,20	0
3	CL	D	1176	1/1	0.96	0.23	15,15,15,15	0
2	MN3	I	1173	1/1	0.97	0.10	26,26,26,26	0
2	MN3	C	1173	1/1	0.98	0.12	30,30,30,30	0
2	MN3	E	1174	1/1	0.98	0.12	29,29,29,29	0
2	MN3	H	1173	1/1	0.98	0.13	24,24,24,24	0
3	CL	A	1174	1/1	0.98	0.19	20,20,20,20	0
2	MN3	J	1173	1/1	0.99	0.19	17,17,17,17	0
5	CA	F	1174	1/1	0.99	0.14	13,13,13,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.