



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 09:33 am GMT

PDB ID : 2V15
Title : Terbium binding in Streptococcus suis Dpr protein
Authors : Havukainen, H.; Papageorgiou, A.C.; Kauko, A.
Deposited on : 2007-05-22
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

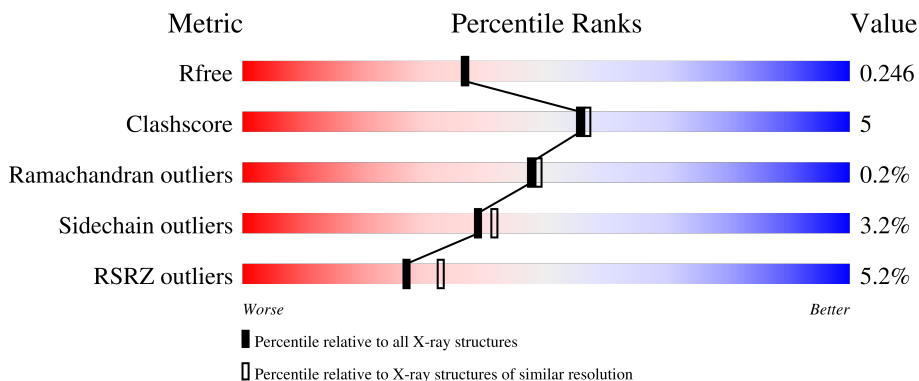
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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	 5% 81% 10% • 8%
1	B	165	 4% 78% 12% • 8%
1	C	165	 5% 81% 11% • 8%
1	D	165	 2% 80% 11% • 8%
1	E	165	 4% 81% 10% • 8%

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Mol	Chain	Length	Quality of chain
1	F	165	
1	G	165	
1	H	165	
1	I	165	
1	J	165	
1	K	165	
1	L	165	

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	C	1173	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15214 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
			Total	C	N	O	S			
1	A	151	1205	768	198	233	6	0	0	0
1	B	151	1205	769	199	231	6	0	0	0
1	C	151	1205	768	198	233	6	0	0	0
1	D	152	1207	769	199	233	6	0	0	0
1	E	151	1189	759	197	227	6	0	0	0
1	F	152	1199	764	198	231	6	0	0	0
1	G	165	1277	812	212	247	6	0	0	0
1	H	152	1185	756	195	228	6	0	0	0
1	I	153	1212	772	200	234	6	0	0	0
1	J	152	1211	771	199	235	6	0	0	0
1	K	152	1207	769	199	233	6	0	0	0
1	L	152	1207	769	199	233	6	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Cl 2	0	0
2	E	2	Total 2	Cl 2	0	0
2	H	1	Total 1	Cl 1	0	0
2	I	2	Total 2	Cl 2	0	0
2	J	1	Total 1	Cl 1	0	0

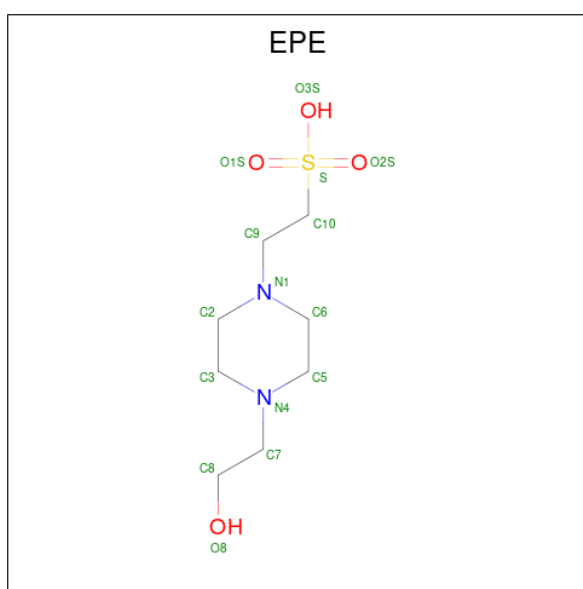
- Molecule 3 is TERBIUM(III) ION (three-letter code: TB) (formula: Tb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Tb 1	0	0
3	B	1	Total 1	Tb 1	0	0
3	C	1	Total 1	Tb 1	0	0
3	D	1	Total 1	Tb 1	0	0
3	E	1	Total 1	Tb 1	0	0
3	F	1	Total 1	Tb 1	0	0
3	G	1	Total 1	Tb 1	0	0
3	H	1	Total 1	Tb 1	0	0
3	I	1	Total 1	Tb 1	0	0
3	J	1	Total 1	Tb 1	0	0
3	K	1	Total 1	Tb 1	0	0
3	L	1	Total 1	Tb 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	G	1	Total Ca 1 1	0	0
4	H	1	Total Ca 1 1	0	0
4	K	1	Total Ca 1 1	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	53	Total O 53 53	0	0

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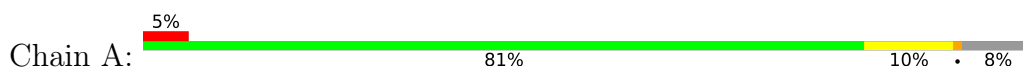
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	59	Total O 59 59	0	0
6	C	45	Total O 45 45	0	0
6	D	66	Total O 66 66	0	0
6	E	37	Total O 37 37	0	0
6	F	61	Total O 61 61	0	0
6	G	53	Total O 53 53	0	0
6	H	40	Total O 40 40	0	0
6	I	57	Total O 57 57	0	0
6	J	46	Total O 46 46	0	0
6	K	59	Total O 59 59	0	0
6	L	43	Total O 43 43	0	0

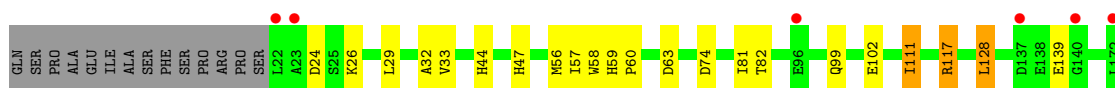
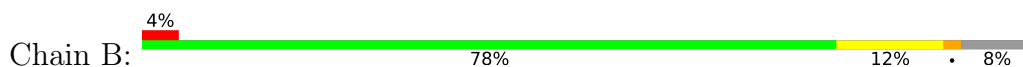
3 Residue-property plots [i](#)

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.

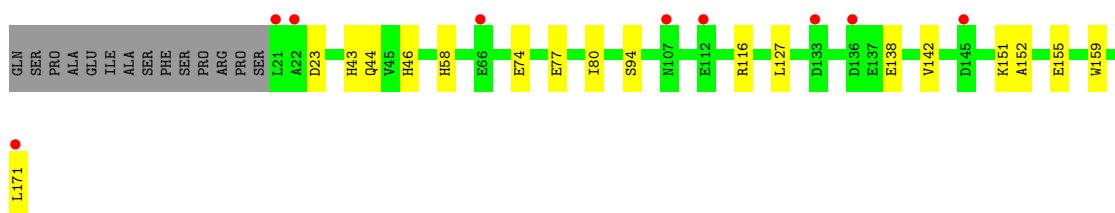
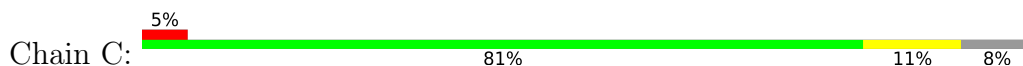
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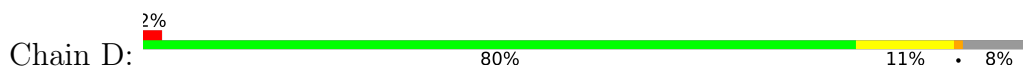
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



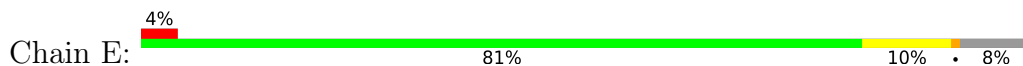
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



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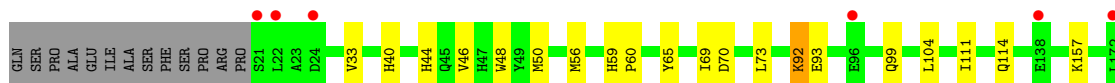
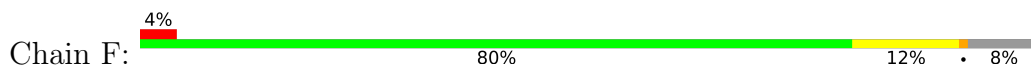


- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

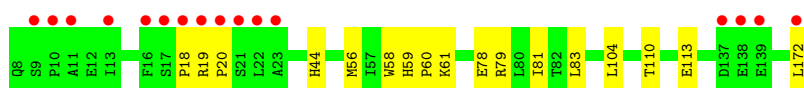
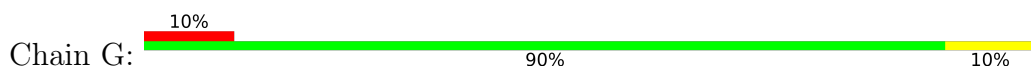




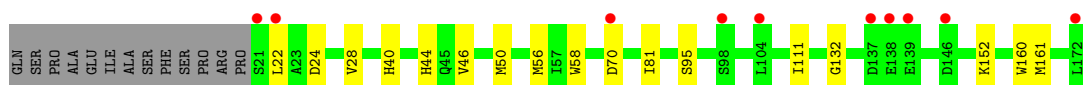
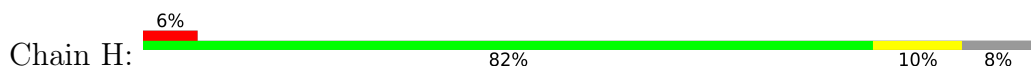
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



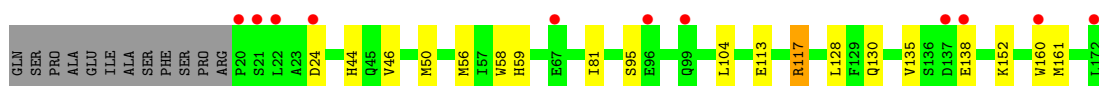
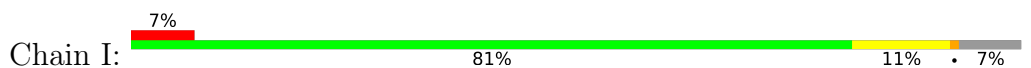
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



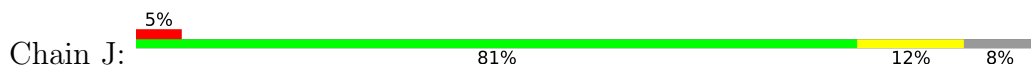
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



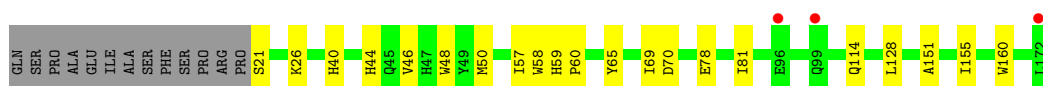
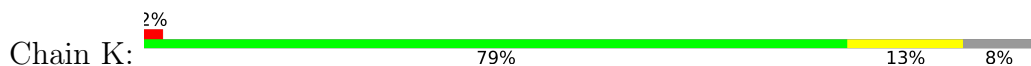
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



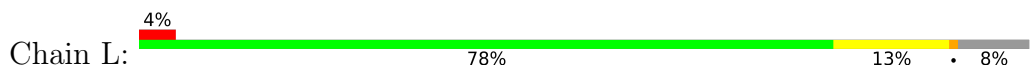
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

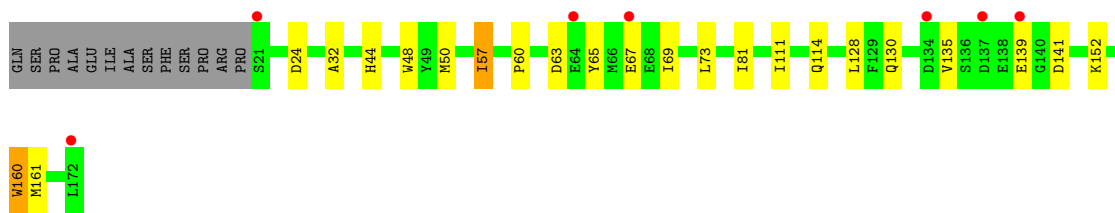


- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



- 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	104.48Å 137.72Å 142.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.10 19.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.10) 96.1 (19.97-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.09Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.244 0.191 , 0.246	Depositor DCC
R_{free} test set	5761 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.038 for -h,l,k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15214	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.29% 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 i

5.1 Standard geometry i

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

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	0.76	1/1230 (0.1%)	0.69	0/1662
1	B	0.75	0/1230	0.75	1/1661 (0.1%)
1	C	0.71	0/1230	0.69	0/1662
1	D	0.78	1/1232 (0.1%)	0.73	1/1665 (0.1%)
1	E	0.66	0/1214	0.71	0/1643
1	F	0.73	0/1224	0.68	0/1656
1	G	0.73	0/1304	0.70	0/1765
1	H	0.70	0/1210	0.68	0/1639
1	I	0.73	0/1237	0.68	0/1672
1	J	0.72	0/1236	0.70	0/1670
1	K	0.72	0/1232	0.68	0/1665
1	L	0.72	0/1232	0.68	1/1665 (0.1%)
All	All	0.72	2/14811 (0.0%)	0.70	3/20025 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	120	GLU	CG-CD	6.56	1.61	1.51
1	A	113	GLU	CG-CD	5.84	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	ASP	CB-CG-OD1	5.72	123.45	118.30
1	L	141	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	141	ASP	CB-CG-OD1	5.07	122.87	118.30

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	1205	0	1163	14	0
1	B	1205	0	1170	18	0
1	C	1205	0	1163	13	0
1	D	1207	0	1164	16	0
1	E	1189	0	1140	12	0
1	F	1199	0	1149	11	0
1	G	1277	0	1199	14	0
1	H	1185	0	1122	12	0
1	I	1212	0	1166	11	0
1	J	1211	0	1168	18	0
1	K	1207	0	1164	14	0
1	L	1207	0	1164	20	0
2	A	1	0	0	0	0
2	C	1	0	0	3	0
2	D	2	0	0	2	0
2	E	2	0	0	0	0
2	H	1	0	0	0	0
2	I	2	0	0	1	0
2	J	1	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	B	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
5	D	15	0	17	0	0
5	E	15	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	15	0	17	1	0
5	K	15	0	17	1	0
6	A	53	0	0	3	0
6	B	59	0	0	2	0
6	C	45	0	0	0	0
6	D	66	0	0	4	0
6	E	37	0	0	0	0
6	F	61	0	0	0	0
6	G	53	0	0	0	0
6	H	40	0	0	0	0
6	I	57	0	0	0	0
6	J	46	0	0	0	0
6	K	59	0	0	0	0
6	L	43	0	0	2	0
All	All	15214	0	14000	146	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 (146) 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)
6:A:2018:HOH:O	2:C:1173:CL:CL	2.13	1.04
1:B:117:ARG:HH11	1:B:117:ARG:HG2	1.31	0.94
2:D:1174:CL:CL	6:D:2025:HOH:O	2.27	0.88
1:J:43:LEU:HD22	1:J:62:MET:HE3	1.57	0.86
1:G:59:HIS:HB3	1:G:60:PRO:HD3	1.58	0.85
1:E:59:HIS:HB3	1:E:60:PRO:HD3	1.63	0.79
1:K:59:HIS:HB3	1:K:60:PRO:HD3	1.66	0.78
1:E:56:MET:HG3	1:L:57:ILE:HD11	1.64	0.78
1:F:59:HIS:HB3	1:F:60:PRO:HD3	1.67	0.76
1:C:58:HIS:HE1	2:C:1173:CL:CL	2.07	0.74
1:K:151:ALA:O	1:K:155:ILE:HG12	1.87	0.74
1:J:43:LEU:CD2	1:J:62:MET:CE	2.66	0.73
1:J:43:LEU:HD22	1:J:62:MET:CE	2.19	0.73
1:D:54:GLY:HA2	6:D:2017:HOH:O	1.89	0.73
1:I:59:HIS:NE2	2:I:1173:CL:CL	2.58	0.72
1:F:114:GLN:HA	1:F:114:GLN:OE1	1.89	0.71
1:C:23:ASP:HB2	1:C:138:GLU:OE2	1.91	0.71
1:J:43:LEU:HD23	1:J:62:MET:HE1	1.73	0.70
1:J:43:LEU:CD2	1:J:62:MET:HE3	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLU:HA	1:C:80:ILE:HD12	1.77	0.65
1:L:24:ASP:HB3	1:L:135:VAL:CG1	2.27	0.65
1:J:43:LEU:CD2	1:J:62:MET:HE1	2.26	0.64
1:K:59:HIS:HB3	1:K:60:PRO:CD	2.26	0.64
1:E:78:GLU:HG2	1:I:160:TRP:CH2	2.33	0.64
1:G:59:HIS:HB3	1:G:60:PRO:CD	2.27	0.64
1:J:81:ILE:HD11	1:L:48:TRP:HB3	1.81	0.62
1:L:50:MET:HG2	1:L:111:ILE:CD1	2.29	0.61
1:K:65:TYR:O	1:K:69:ILE:HG12	2.00	0.61
1:G:78:GLU:HG2	1:L:160:TRP:CH2	2.36	0.61
1:J:59:HIS:HB3	1:J:60:PRO:HD3	1.83	0.61
1:L:24:ASP:HB3	1:L:135:VAL:HG11	1.82	0.61
1:J:43:LEU:HD23	1:J:62:MET:CE	2.31	0.60
1:E:130:GLN:OE1	1:E:152:LYS:HE2	2.02	0.59
1:L:114:GLN:HA	1:L:114:GLN:OE1	2.03	0.59
1:J:48:TRP:HB3	1:L:81:ILE:HD11	1.85	0.58
1:F:40:HIS:CD2	1:F:70:ASP:OD1	2.57	0.57
1:B:81:ILE:HD11	1:D:48:TRP:HB3	1.87	0.57
1:C:77:GLU:HG2	1:H:160:TRP:CH2	2.41	0.56
1:A:56:MET:HE3	1:H:58:TRP:CH2	2.40	0.56
1:B:82:THR:HG22	1:G:172:LEU:HD11	1.88	0.56
1:B:117:ARG:HH11	1:B:117:ARG:CG	2.13	0.56
1:D:61:LYS:HE3	1:D:64:GLU:OE1	2.05	0.56
1:C:58:HIS:CE1	2:C:1173:CL:CL	2.93	0.55
6:D:2029:HOH:O	1:F:157:LYS:HE2	2.05	0.55
1:E:114:GLN:HA	1:E:114:GLN:OE1	2.07	0.55
1:K:21:SER:O	1:K:26:LYS:HE2	2.07	0.55
1:A:108:ASN:ND2	6:A:2033:HOH:O	2.12	0.54
1:D:59:HIS:HE1	2:D:1175:CL:CL	2.28	0.53
1:E:56:MET:HE1	1:L:161:MET:HB3	1.89	0.53
1:G:110:THR:OG1	1:G:113:GLU:HG3	2.09	0.53
1:B:60:PRO:O	1:B:63:ASP:HB2	2.09	0.52
1:A:78:GLU:HG2	1:E:160:TRP:CH2	2.45	0.52
1:C:44:GLN:OE1	1:C:116:ARG:NH2	2.42	0.52
1:A:82:THR:HG22	1:E:172:LEU:HD11	1.92	0.52
1:J:130:GLN:OE1	1:J:152:LYS:HE3	2.10	0.51
1:E:92:LYS:O	1:E:96:GLU:HG3	2.10	0.51
1:L:32:ALA:HA	1:L:128:LEU:HD21	1.91	0.51
1:I:46:VAL:O	1:I:50:MET:HB2	2.11	0.51
1:E:48:TRP:HB3	1:G:81:ILE:HD11	1.93	0.51
1:B:117:ARG:HG2	1:B:117:ARG:NH1	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:GLN:HB2	1:I:152:LYS:HE3	1.93	0.51
1:H:40:HIS:CD2	1:H:70:ASP:OD2	2.64	0.50
1:L:50:MET:HG2	1:L:111:ILE:HD11	1.92	0.50
1:H:28:VAL:HG21	1:H:132:GLY:HA2	1.93	0.49
1:B:59:HIS:HB3	1:B:60:PRO:CD	2.41	0.49
1:L:50:MET:HG2	1:L:111:ILE:HD13	1.94	0.49
1:B:59:HIS:HB3	1:B:60:PRO:HD3	1.94	0.49
1:K:40:HIS:CD2	1:K:70:ASP:OD2	2.66	0.49
1:D:47:HIS:O	1:D:59:HIS:HD2	1.96	0.48
1:F:92:LYS:HG3	1:F:93:GLU:N	2.28	0.48
1:G:56:MET:HE1	1:I:161:MET:HB3	1.96	0.47
1:H:56:MET:HE2	1:K:58:TRP:CH2	2.49	0.47
1:K:59:HIS:CB	1:K:60:PRO:HD3	2.42	0.47
1:B:29:LEU:O	1:B:33:VAL:HG23	2.15	0.47
1:I:24:ASP:HB3	1:I:135:VAL:HG11	1.96	0.47
1:L:60:PRO:O	1:L:63:ASP:HB2	2.14	0.47
1:D:56:MET:CE	1:G:58:TRP:CH2	2.98	0.47
1:H:46:VAL:O	1:H:50:MET:HB2	2.14	0.47
1:A:56:MET:HE1	1:H:161:MET:HB3	1.97	0.46
1:K:46:VAL:O	1:K:50:MET:HB2	2.16	0.46
1:B:111:ILE:HG22	6:B:2039:HOH:O	2.14	0.46
1:F:56:MET:HE1	1:J:161:MET:HB3	1.97	0.46
1:J:59:HIS:NE2	2:J:1173:CL:CL	2.78	0.46
1:B:102:GLU:HB3	1:D:90:THR:HG22	1.98	0.46
1:D:56:MET:HE2	1:G:58:TRP:CH2	2.51	0.46
1:J:92:LYS:HB2	6:L:2027:HOH:O	2.15	0.46
1:A:56:MET:CE	1:H:58:TRP:CH2	2.99	0.46
1:C:171:LEU:HD11	1:J:82:THR:HG22	1.98	0.46
1:A:130:GLN:OE1	1:A:152:LYS:HE3	2.15	0.45
1:B:26:LYS:HG3	6:B:2002:HOH:O	2.16	0.45
1:L:24:ASP:HB3	1:L:135:VAL:HG13	1.98	0.45
1:D:32:ALA:HB2	1:D:128:LEU:HD11	1.98	0.45
1:L:65:TYR:O	1:L:69:ILE:HG12	2.16	0.45
1:L:24:ASP:HB2	1:L:139:GLU:OE2	2.16	0.45
1:C:142:VAL:HG23	1:H:152:LYS:NZ	2.31	0.45
1:C:151:LYS:HE2	1:C:155:GLU:OE2	2.16	0.45
1:B:24:ASP:HB2	1:B:139:GLU:OE2	2.16	0.45
1:B:58:TRP:CH2	1:J:56:MET:HE3	2.52	0.44
1:K:57:ILE:HG23	1:K:58:TRP:CD1	2.52	0.44
1:B:32:ALA:HA	1:B:128:LEU:HD11	1.99	0.44
1:K:59:HIS:CB	1:K:60:PRO:CD	2.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLY:HA2	6:A:2021:HOH:O	2.16	0.44
1:A:109:VAL:HG12	1:A:114:GLN:HG2	1.98	0.44
1:G:59:HIS:CB	1:G:60:PRO:HD3	2.39	0.44
1:J:29:LEU:HD21	1:J:144:THR:HG23	2.00	0.44
1:B:24:ASP:CB	1:B:139:GLU:OE2	2.66	0.44
1:G:79:ARG:NH2	1:G:83:LEU:HD21	2.33	0.44
1:K:114:GLN:HA	1:K:114:GLN:OE1	2.18	0.44
1:I:135:VAL:O	1:I:138:GLU:HB2	2.17	0.44
5:K:1174:EPE:H81	5:K:1174:EPE:H31	1.76	0.43
1:A:109:VAL:HG13	1:A:113:GLU:HB3	2.00	0.43
1:G:56:MET:HE3	1:I:58:TRP:CH2	2.52	0.43
1:C:46:HIS:CE1	1:C:58:HIS:CE1	3.07	0.43
5:F:1174:EPE:H21	5:F:1174:EPE:H102	1.80	0.43
1:C:46:HIS:CE1	1:C:58:HIS:NE2	2.87	0.43
1:K:78:GLU:HA	1:K:81:ILE:HD12	2.01	0.43
1:L:130:GLN:OE1	1:L:152:LYS:HE3	2.18	0.43
1:B:56:MET:HB2	1:B:56:MET:HE2	1.95	0.43
1:C:152:ALA:HB2	1:J:143:VAL:HG13	2.01	0.43
1:I:81:ILE:HD11	1:K:48:TRP:HB3	2.00	0.43
1:C:151:LYS:NZ	1:C:155:GLU:OE2	2.49	0.42
1:B:47:HIS:CE1	1:B:59:HIS:CE1	3.07	0.42
1:D:58:TRP:CH2	1:I:56:MET:HE3	2.54	0.42
1:G:61:LYS:HA	1:G:61:LYS:HD3	1.86	0.42
1:A:109:VAL:CG1	1:A:113:GLU:HB3	2.50	0.42
1:A:57:ILE:HG23	1:A:58:TRP:CD1	2.54	0.42
1:H:28:VAL:HG21	1:H:132:GLY:CA	2.49	0.42
1:A:28:VAL:HG11	1:A:132:GLY:HA2	2.01	0.42
1:D:155:ILE:HA	1:D:155:ILE:HD13	1.73	0.42
1:F:99:GLN:HE21	1:F:99:GLN:HB3	1.65	0.42
1:D:46:VAL:O	1:D:50:MET:HB2	2.20	0.42
1:F:46:VAL:O	1:F:50:MET:HB2	2.20	0.42
1:F:48:TRP:HB3	1:H:81:ILE:HD11	2.01	0.41
1:A:56:MET:CE	1:H:58:TRP:HH2	2.33	0.41
1:F:33:VAL:HG13	1:F:73:LEU:HD11	2.02	0.41
1:F:65:TYR:O	1:F:69:ILE:HG12	2.21	0.41
1:D:47:HIS:O	1:D:59:HIS:CD2	2.74	0.41
1:D:54:GLY:CA	6:D:2017:HOH:O	2.59	0.41
1:D:59:HIS:HB3	1:D:60:PRO:CD	2.50	0.41
1:L:57:ILE:HD12	6:L:2010:HOH:O	2.21	0.41
1:E:40:HIS:CD2	1:E:70:ASP:OD1	2.74	0.40
1:D:116:ALA:O	1:D:120:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:50:MET:CG	1:L:111:ILE:HD13	2.51	0.40
1:E:56:MET:CG	1:L:57:ILE:HD11	2.44	0.40
1:G:59:HIS:CB	1:G:60:PRO:CD	2.94	0.40
1:I:113:GLU:O	1:I:117:ARG:HG3	2.21	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	149/165 (90%)	148 (99%)	1 (1%)	0	100	100
1	B	149/165 (90%)	147 (99%)	2 (1%)	0	100	100
1	C	149/165 (90%)	148 (99%)	1 (1%)	0	100	100
1	D	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	E	149/165 (90%)	147 (99%)	2 (1%)	0	100	100
1	F	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	G	163/165 (99%)	158 (97%)	2 (1%)	3 (2%)	8	4
1	H	150/165 (91%)	147 (98%)	2 (1%)	1 (1%)	22	18
1	I	151/165 (92%)	150 (99%)	1 (1%)	0	100	100
1	J	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	K	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	L	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
All	All	1810/1980 (91%)	1790 (99%)	16 (1%)	4 (0%)	47	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	19	ARG
1	G	20	PRO
1	H	22	LEU
1	G	18	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	128/141 (91%)	125 (98%)	3 (2%)	50 55
1	B	128/141 (91%)	122 (95%)	6 (5%)	26 25
1	C	128/141 (91%)	123 (96%)	5 (4%)	32 33
1	D	128/141 (91%)	125 (98%)	3 (2%)	50 55
1	E	124/141 (88%)	119 (96%)	5 (4%)	31 32
1	F	126/141 (89%)	122 (97%)	4 (3%)	39 41
1	G	130/141 (92%)	128 (98%)	2 (2%)	65 71
1	H	122/141 (86%)	118 (97%)	4 (3%)	38 40
1	I	128/141 (91%)	123 (96%)	5 (4%)	32 33
1	J	129/141 (92%)	125 (97%)	4 (3%)	40 43
1	K	128/141 (91%)	125 (98%)	3 (2%)	50 55
1	L	128/141 (91%)	123 (96%)	5 (4%)	32 33
All	All	1527/1692 (90%)	1478 (97%)	49 (3%)	39 41

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	95	SER
1	A	160	TRP
1	B	44	HIS
1	B	57	ILE
1	B	99	GLN
1	B	111	ILE

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Mol	Chain	Res	Type
1	B	117	ARG
1	B	128	LEU
1	C	43	HIS
1	C	74	GLU
1	C	94	SER
1	C	127	LEU
1	C	159	TRP
1	D	57	ILE
1	D	61	LYS
1	D	160	TRP
1	E	22	LEU
1	E	24	ASP
1	E	44	HIS
1	E	95	SER
1	E	160	TRP
1	F	44	HIS
1	F	92	LYS
1	F	104	LEU
1	F	111	ILE
1	G	44	HIS
1	G	104	LEU
1	H	24	ASP
1	H	44	HIS
1	H	95	SER
1	H	111	ILE
1	I	44	HIS
1	I	95	SER
1	I	104	LEU
1	I	117	ARG
1	I	128	LEU
1	J	44	HIS
1	J	95	SER
1	J	128	LEU
1	J	160	TRP
1	K	44	HIS
1	K	128	LEU
1	K	160	TRP
1	L	44	HIS
1	L	57	ILE
1	L	67	GLU
1	L	73	LEU
1	L	160	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	58	HIS
1	D	59	HIS
1	D	145	ASN
1	E	40	HIS
1	F	40	HIS
1	F	59	HIS
1	F	99	GLN
1	F	145	ASN
1	G	40	HIS
1	H	40	HIS
1	H	108	ASN
1	I	99	GLN
1	I	145	ASN
1	J	99	GLN
1	K	40	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 26 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
5	EPE	E	1173	-	15,15,15	0.89	1 (6%)	18,20,20	2.23	6 (33%)
5	EPE	K	1174	-	15,15,15	1.00	1 (6%)	18,20,20	2.07	6 (33%)
5	EPE	F	1174	-	15,15,15	0.76	1 (6%)	18,20,20	2.05	4 (22%)
5	EPE	D	1176	-	15,15,15	0.67	0	18,20,20	2.20	7 (38%)

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
5	EPE	E	1173	-	-	6/9/19/19	0/1/1/1
5	EPE	K	1174	-	-	7/9/19/19	0/1/1/1
5	EPE	F	1174	-	-	7/9/19/19	0/1/1/1
5	EPE	D	1176	-	-	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)
5	K	1174	EPE	C10-S	3.56	1.82	1.77
5	E	1173	EPE	C10-S	3.10	1.81	1.77
5	F	1174	EPE	C10-S	2.30	1.80	1.77

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1174	EPE	O1S-S-C10	5.91	114.03	106.92
5	E	1173	EPE	C5-N4-C3	5.47	121.13	108.83
5	D	1176	EPE	O1S-S-C10	5.00	112.94	106.92
5	D	1176	EPE	C5-N4-C3	4.48	118.91	108.83
5	F	1174	EPE	C5-N4-C3	4.09	118.03	108.83
5	K	1174	EPE	C7-N4-C3	3.99	121.45	111.23
5	E	1173	EPE	O3S-S-C10	3.96	112.17	105.77
5	K	1174	EPE	O1S-S-C10	3.88	111.58	106.92
5	K	1174	EPE	C5-N4-C3	3.34	116.34	108.83
5	E	1173	EPE	C7-N4-C5	3.13	119.23	111.23
5	E	1173	EPE	C7-N4-C3	3.12	119.20	111.23
5	K	1174	EPE	O3S-S-C10	3.10	110.77	105.77
5	D	1176	EPE	C7-N4-C3	3.01	118.93	111.23
5	F	1174	EPE	C7-N4-C5	2.98	118.86	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1176	EPE	C7-N4-C5	2.84	118.49	111.23
5	K	1174	EPE	O2S-S-C10	2.77	110.25	106.92
5	F	1174	EPE	C7-N4-C3	2.74	118.23	111.23
5	K	1174	EPE	C7-N4-C5	2.54	117.73	111.23
5	E	1173	EPE	O2S-S-C10	2.51	109.94	106.92
5	D	1176	EPE	O3S-S-O1S	-2.37	105.47	111.27
5	D	1176	EPE	C9-N1-C2	-2.30	105.35	111.23
5	E	1173	EPE	C6-C5-N4	2.26	115.28	110.64
5	D	1176	EPE	O3S-S-C10	2.24	109.39	105.77

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1176	EPE	C10-C9-N1-C2
5	D	1176	EPE	C10-C9-N1-C6
5	E	1173	EPE	C10-C9-N1-C6
5	E	1173	EPE	C9-C10-S-O1S
5	E	1173	EPE	C9-C10-S-O3S
5	F	1174	EPE	C10-C9-N1-C2
5	K	1174	EPE	C10-C9-N1-C2
5	K	1174	EPE	C10-C9-N1-C6
5	K	1174	EPE	C8-C7-N4-C3
5	K	1174	EPE	C9-C10-S-O2S
5	K	1174	EPE	C9-C10-S-O3S
5	E	1173	EPE	N4-C7-C8-O8
5	K	1174	EPE	N4-C7-C8-O8
5	F	1174	EPE	C9-C10-S-O3S
5	E	1173	EPE	C8-C7-N4-C3
5	F	1174	EPE	C8-C7-N4-C3
5	E	1173	EPE	C9-C10-S-O2S
5	F	1174	EPE	C9-C10-S-O1S
5	F	1174	EPE	C9-C10-S-O2S
5	K	1174	EPE	C9-C10-S-O1S
5	F	1174	EPE	C10-C9-N1-C6
5	D	1176	EPE	C8-C7-N4-C3
5	D	1176	EPE	C8-C7-N4-C5
5	F	1174	EPE	C8-C7-N4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1174	EPE	1	0
5	F	1174	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%)	0.30	8 (5%) 26 32	25, 32, 43, 49	0
1	B	151/165 (91%)	0.26	6 (3%) 38 44	22, 30, 41, 59	1 (0%)
1	C	151/165 (91%)	0.30	9 (5%) 21 27	28, 35, 47, 62	1 (0%)
1	D	152/165 (92%)	0.09	3 (1%) 65 69	22, 29, 41, 51	0
1	E	151/165 (91%)	0.32	7 (4%) 32 38	27, 35, 45, 61	0
1	F	152/165 (92%)	0.16	6 (3%) 39 45	22, 30, 43, 60	0
1	G	165/165 (100%)	0.54	16 (9%) 7 10	24, 34, 61, 76	0
1	H	152/165 (92%)	0.28	10 (6%) 18 23	24, 34, 48, 60	0
1	I	153/165 (92%)	0.34	11 (7%) 15 19	23, 32, 44, 66	0
1	J	152/165 (92%)	0.34	9 (5%) 22 27	26, 34, 46, 56	0
1	K	152/165 (92%)	0.17	3 (1%) 65 69	23, 30, 41, 45	0
1	L	152/165 (92%)	0.32	7 (4%) 32 38	26, 34, 46, 53	0
All	All	1834/1980 (92%)	0.29	95 (5%) 27 32	22, 33, 46, 76	2 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	18	PRO	9.7
1	E	23	ALA	7.4
1	G	19	ARG	7.0
1	I	20	PRO	6.9
1	B	172	LEU	6.4
1	G	172	LEU	6.1
1	B	23	ALA	6.0
1	C	22	ALA	6.0
1	G	17	SER	5.5
1	B	22	LEU	5.3
1	H	137	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	G	20	PRO	5.1
1	J	172	LEU	5.1
1	H	21	SER	5.0
1	E	172	LEU	4.9
1	H	172	LEU	4.9
1	L	172	LEU	4.7
1	A	172	LEU	4.6
1	I	172	LEU	4.6
1	C	171	LEU	4.6
1	D	172	LEU	4.5
1	E	22	LEU	4.4
1	C	21	LEU	4.3
1	F	21	SER	4.3
1	G	10	PRO	4.2
1	G	21	SER	3.9
1	A	23	ALA	3.8
1	A	22	LEU	3.7
1	L	21	SER	3.6
1	K	172	LEU	3.4
1	G	137	ASP	3.3
1	G	11	ALA	3.2
1	J	21	SER	3.2
1	F	22	LEU	3.2
1	B	96	GLU	3.2
1	G	138	GLU	3.1
1	H	139	GLU	3.1
1	I	21	SER	3.1
1	I	137	ASP	3.0
1	D	21	SER	2.9
1	C	66	GLU	2.9
1	J	137	ASP	2.9
1	G	22	LEU	2.8
1	K	96	GLU	2.8
1	F	172	LEU	2.8
1	E	96	GLU	2.7
1	E	134	ASP	2.7
1	E	70	ASP	2.6
1	F	96	GLU	2.6
1	L	139	GLU	2.6
1	I	22	LEU	2.6
1	L	134	ASP	2.6
1	B	137	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	138	GLU	2.6
1	G	9	SER	2.5
1	H	138	GLU	2.5
1	G	16	PHE	2.5
1	L	137	ASP	2.5
1	A	162	LEU	2.5
1	F	24	ASP	2.5
1	F	138	GLU	2.4
1	H	98	SER	2.4
1	B	140	GLY	2.4
1	C	112	GLU	2.4
1	J	96	GLU	2.4
1	A	138	GLU	2.4
1	C	107	ASN	2.4
1	K	99	GLN	2.4
1	J	146	ASP	2.4
1	J	138	GLU	2.4
1	A	141	ASP	2.3
1	G	139	GLU	2.3
1	E	137	ASP	2.3
1	J	134	ASP	2.3
1	C	136	ASP	2.2
1	G	23	ALA	2.2
1	I	67	GLU	2.2
1	L	67	GLU	2.2
1	D	134	ASP	2.2
1	H	146	ASP	2.2
1	A	99	GLN	2.1
1	A	67	GLU	2.1
1	J	22	LEU	2.1
1	I	160	TRP	2.1
1	I	96	GLU	2.1
1	J	67	GLU	2.1
1	C	133	ASP	2.0
1	H	22	LEU	2.0
1	H	70	ASP	2.0
1	G	13	ILE	2.0
1	H	104	LEU	2.0
1	C	145	ASP	2.0
1	I	24	ASP	2.0
1	L	64	GLU	2.0
1	I	99	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EPE	K	1174	15/15	0.88	0.20	62,69,72,72	0
5	EPE	F	1174	15/15	0.89	0.20	56,66,74,75	0
5	EPE	E	1173	15/15	0.89	0.17	61,67,75,75	0
5	EPE	D	1176	15/15	0.92	0.18	42,43,48,49	10
4	CA	B	1173	1/1	0.92	0.20	58,58,58,58	0
2	CL	I	1175	1/1	0.93	0.07	52,52,52,52	0
2	CL	E	1176	1/1	0.93	0.11	47,47,47,47	0
4	CA	G	173	1/1	0.95	0.09	74,74,74,74	0
4	CA	K	1175	1/1	0.95	0.04	36,36,36,36	0
2	CL	C	1173	1/1	0.96	0.07	46,46,46,46	0
2	CL	J	1173	1/1	0.96	0.20	49,49,49,49	0
2	CL	I	1173	1/1	0.96	0.10	47,47,47,47	0
2	CL	D	1174	1/1	0.97	0.10	47,47,47,47	0
2	CL	D	1175	1/1	0.97	0.06	49,49,49,49	0
4	CA	H	1174	1/1	0.97	0.11	28,28,28,28	1
2	CL	A	1173	1/1	0.97	0.10	48,48,48,48	0
2	CL	H	1175	1/1	0.98	0.06	49,49,49,49	0
2	CL	E	1174	1/1	0.99	0.10	55,55,55,55	0
3	TB	I	1174	1/1	1.00	0.02	33,33,33,33	0
3	TB	J	1174	1/1	1.00	0.02	36,36,36,36	0
3	TB	K	1173	1/1	1.00	0.02	29,29,29,29	0
3	TB	L	1173	1/1	1.00	0.02	33,33,33,33	0
3	TB	A	1174	1/1	1.00	0.02	33,33,33,33	0
3	TB	B	1174	1/1	1.00	0.02	30,30,30,30	0
3	TB	C	1172	1/1	1.00	0.02	34,34,34,34	0
3	TB	D	1173	1/1	1.00	0.02	31,31,31,31	0
3	TB	E	1175	1/1	1.00	0.02	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TB	F	1173	1/1	1.00	0.02	32,32,32,32	0
3	TB	G	1173	1/1	1.00	0.01	36,36,36,36	0
3	TB	H	1173	1/1	1.00	0.02	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.