



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:42 PM UTC

PDB ID : 2CF7 / pdb_00002cf7
Title : Asp74Ala mutant crystal structure for Dps-like peroxide resistance protein Dpr from *Streptococcus suis*.
Authors : Kauko, A.; Pulliainen, A.T.; Haataja, S.; Finne, J.; Papageorgiou, A.C.
Deposited on : 2006-02-16
Resolution : 1.50 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

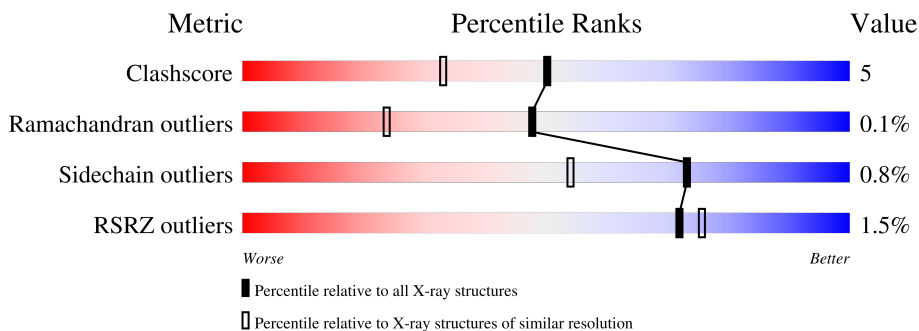
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	
1	F	165	

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Mol	Chain	Length	Quality of chain
1	G	165	 88% 5% 7% 2%
1	H	165	 86% 5% 8% 2%
1	I	165	 85% 7% 8% 2%
1	J	165	 86% 5% 8% 2%
1	K	165	 89% 5% 8% 2%
1	L	165	 82% 10% 8% 2%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 17112 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 DPR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1274	821	205	241	7	0	9	0
1	B	150	1238	799	201	231	7	0	11	0
1	C	152	1246	802	198	239	7	0	10	0
1	D	152	1227	787	199	234	7	0	6	0
1	E	151	1245	804	198	236	7	0	10	0
1	F	151	1249	807	201	235	6	0	10	0
1	G	153	1240	795	199	239	7	0	7	0
1	H	151	1281	831	199	244	7	0	15	0
1	I	152	1249	807	200	235	7	0	10	0
1	J	151	1246	802	203	234	7	0	11	0
1	K	151	1228	785	199	237	7	0	6	0
1	L	151	1231	792	199	233	7	0	8	0

There are 12 discrepancies between the modelled and reference sequences:

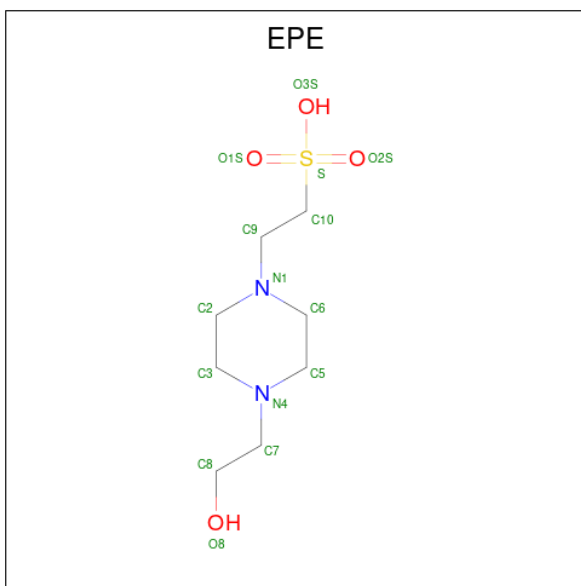
Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	ASP	engineered mutation	UNP Q9F5J9
B	74	ALA	ASP	engineered mutation	UNP Q9F5J9
C	74	ALA	ASP	engineered mutation	UNP Q9F5J9
D	74	ALA	ASP	engineered mutation	UNP Q9F5J9
E	74	ALA	ASP	engineered mutation	UNP Q9F5J9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	74	ALA	ASP	engineered mutation	UNP Q9F5J9
G	74	ALA	ASP	engineered mutation	UNP Q9F5J9
H	74	ALA	ASP	engineered mutation	UNP Q9F5J9
I	74	ALA	ASP	engineered mutation	UNP Q9F5J9
J	74	ALA	ASP	engineered mutation	UNP Q9F5J9
K	74	ALA	ASP	engineered mutation	UNP Q9F5J9
L	74	ALA	ASP	engineered mutation	UNP Q9F5J9

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	Total	C	N	O	S	0	1
30	16	4	8	2					
2	E	1	Total	C	N	O	S	0	1
30	16	4	8	2					
2	G	1	Total	C	N	O	S	0	0
15	8	2	4	1					
2	K	1	Total	C	N	O	S	0	1
30	16	4	8	2					

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Ca	0	0
1	1					

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total Ca 1 1	0	0
3	K	1	Total Ca 1 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total Cl 1 1	0	0
4	K	1	Total Cl 1 1	0	0

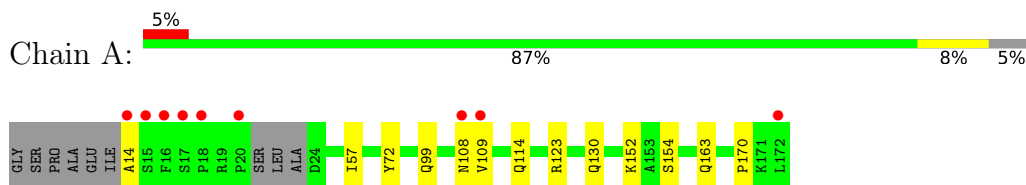
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	169	Total O 169 169	0	0
5	B	179	Total O 179 179	0	0
5	C	170	Total O 170 170	0	0
5	D	183	Total O 183 183	0	0
5	E	153	Total O 153 153	0	0
5	F	183	Total O 183 183	0	0
5	G	153	Total O 153 153	0	0
5	H	182	Total O 182 182	0	0
5	I	166	Total O 166 166	0	0
5	J	179	Total O 179 179	0	0
5	K	187	Total O 187 187	0	0
5	L	144	Total O 144 144	0	0

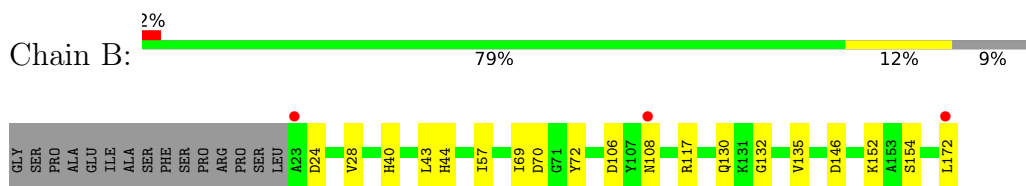
3 Residue-property plots [i](#)

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.

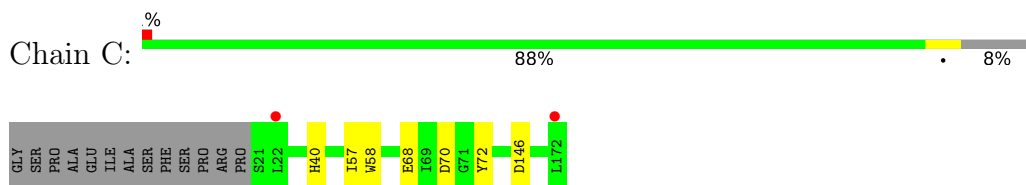
- Molecule 1: DPR



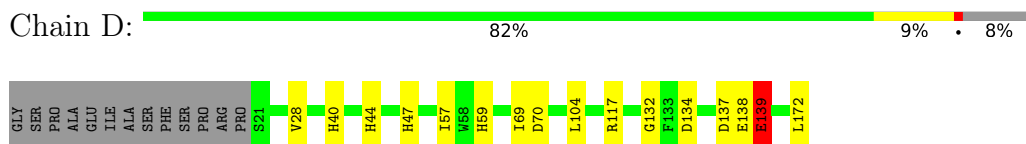
- Molecule 1: DPR



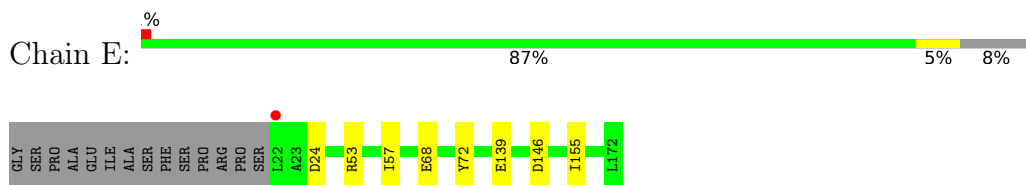
- Molecule 1: DPR




- Molecule 1: DPR



- Molecule 1: DPR




- Molecule 1: DPR

Chain F:  84% 7% 8%




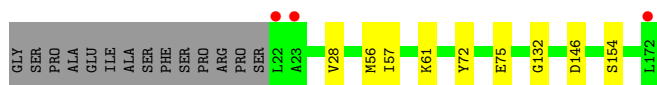
● Molecule 1: DPR

Chain G:  88% 5% 7%




● Molecule 1: DPR

Chain H:  2% 86% 5% 8%




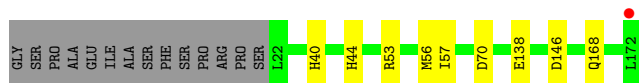
● Molecule 1: DPR

Chain I:  2% 85% 7% 8%




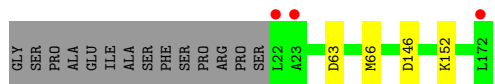
● Molecule 1: DPR

Chain J:  2% 86% 5% 8%




● Molecule 1: DPR

Chain K:  2% 89% 8%



● Molecule 1: DPR

Chain L:  2% 82% 10% 8%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.93Å 133.67Å 135.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.28 – 1.50 19.28 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.28-1.50) 99.9 (19.28-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.153 , 0.177 0.155 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtrriage
Anisotropy	0.036	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.012 for -h,l,k	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17112	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6212e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, EPE, 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	0.78	0/1328	0.82	0/1795
1	B	0.74	0/1296	0.81	0/1750
1	C	0.72	0/1302	0.80	0/1761
1	D	0.81	1/1270 (0.1%)	0.84	0/1718
1	E	0.70	0/1301	0.79	0/1760
1	F	0.76	0/1303	0.82	0/1763
1	G	0.72	0/1287	0.85	1/1741 (0.1%)
1	H	0.76	0/1352	0.85	0/1826
1	I	0.74	0/1305	0.80	0/1765
1	J	0.76	0/1305	0.84	0/1763
1	K	0.82	0/1271	0.85	0/1717
1	L	0.71	0/1281	0.83	0/1732
All	All	0.75	1/15601 (0.0%)	0.83	1/21091 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	139	GLU	CB-CG	6.03	1.70	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	20	PRO	N-CA-CB	6.63	110.29	103.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	138	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1274	0	1252	23	1
1	B	1238	0	1232	34	1
1	C	1246	0	1221	6	0
1	D	1227	0	1197	11	0
1	E	1245	0	1225	9	0
1	F	1249	0	1233	27	0
1	G	1240	0	1203	20	0
1	H	1281	0	1286	23	0
1	I	1249	0	1232	19	0
1	J	1246	0	1229	24	0
1	K	1228	0	1196	5	0
1	L	1231	0	1207	13	0
2	B	30	0	34	1	0
2	E	30	0	34	1	0
2	G	15	0	17	0	0
2	K	30	0	34	1	0
3	D	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
5	A	169	0	0	5	0
5	B	179	0	0	3	0
5	C	170	0	0	1	0
5	D	183	0	0	1	0
5	E	153	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	183	0	0	5	0
5	G	153	0	0	2	0
5	H	182	0	0	7	0
5	I	166	0	0	2	0
5	J	179	0	0	5	0
5	K	187	0	0	3	0
5	L	144	0	0	0	0
All	All	17112	0	14832	159	1

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 (159) 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:F:57[B]:ILE:CD1	1:J:57[B]:ILE:HD11	1.39	1.48
1:B:57[B]:ILE:HD11	1:J:57[B]:ILE:CD1	1.65	1.25
1:B:57[B]:ILE:HD11	1:F:57[B]:ILE:HD11	1.21	1.14
1:F:40[B]:HIS:HD2	5:F:2023:HOH:O	1.30	1.13
1:B:57[B]:ILE:CD1	1:F:57[B]:ILE:HD11	1.78	1.13
1:J:40[B]:HIS:CD2	5:J:2022:HOH:O	2.00	1.10
1:E:57[A]:ILE:HD11	1:L:57[A]:ILE:HD11	1.33	1.06
1:B:57[B]:ILE:HD11	1:J:57[B]:ILE:HD11	1.29	1.05
1:F:57[B]:ILE:CD1	1:J:57[B]:ILE:CD1	2.33	1.05
1:B:57[B]:ILE:CD1	1:J:57[B]:ILE:HG13	1.87	1.04
1:B:57[B]:ILE:HD11	1:J:57[B]:ILE:CG1	1.89	1.02
1:B:57[B]:ILE:CG1	1:F:57[B]:ILE:HD11	1.90	1.01
1:F:40[B]:HIS:CD2	5:F:2023:HOH:O	2.04	1.00
1:F:57[B]:ILE:HD11	1:J:57[B]:ILE:HD11	1.03	0.99
1:F:57[B]:ILE:HD11	1:J:57[B]:ILE:CD1	1.92	0.96
1:J:40[B]:HIS:HD2	5:J:2022:HOH:O	1.40	0.95
1:G:57[B]:ILE:HD11	1:I:57[B]:ILE:HG12	1.49	0.94
1:A:57[B]:ILE:CG1	1:H:57[B]:ILE:HD11	1.97	0.93
1:D:57:ILE:HD11	1:G:57[B]:ILE:CD1	1.99	0.92
1:F:57[B]:ILE:CG1	1:J:57[B]:ILE:HD11	2.00	0.91
1:J:146[A]:ASP:OD1	5:J:2156:HOH:O	1.87	0.91
1:B:57[B]:ILE:HD13	1:J:57[B]:ILE:HG13	1.50	0.91
1:A:57[B]:ILE:HG12	1:H:57[B]:ILE:CD1	2.01	0.91
1:G:57[B]:ILE:HD11	1:I:57[B]:ILE:CD1	2.01	0.90
1:B:57[B]:ILE:HG13	1:F:57[B]:ILE:CD1	2.02	0.89
1:A:57[B]:ILE:HG12	1:H:57[B]:ILE:HD11	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57[B]:ILE:HD12	1:J:57[B]:ILE:HD11	1.52	0.88
1:G:57[B]:ILE:CG1	1:I:57[B]:ILE:HD11	2.04	0.87
1:F:57[B]:ILE:HG13	1:J:57[B]:ILE:CD1	2.05	0.86
1:G:57[B]:ILE:HD11	1:I:57[B]:ILE:CG1	2.04	0.86
1:F:57[B]:ILE:HG13	1:J:57[B]:ILE:HD13	1.58	0.84
1:G:146[A]:ASP:OD1	5:G:2129:HOH:O	1.96	0.83
1:B:57[B]:ILE:CG1	1:F:57[B]:ILE:CD1	2.55	0.83
1:A:14:ALA:HB1	5:A:2002:HOH:O	1.78	0.82
1:B:57[B]:ILE:HG13	1:F:57[B]:ILE:HD13	1.61	0.82
1:B:43:LEU:CD1	1:B:69[B]:ILE:HD12	2.10	0.81
1:K:146[A]:ASP:OD1	5:K:2156:HOH:O	1.98	0.81
1:B:106:ASP:CB	5:B:2119:HOH:O	2.28	0.81
1:B:57[B]:ILE:CD1	1:J:57[B]:ILE:CG1	2.54	0.81
1:F:57[B]:ILE:CG1	1:J:57[B]:ILE:CD1	2.59	0.80
1:B:43:LEU:HD11	1:B:69[B]:ILE:CD1	2.13	0.79
1:B:57[B]:ILE:HD11	1:F:57[B]:ILE:CD1	2.09	0.79
1:I:40:HIS:CE1	1:I:66[B]:MET:HE3	2.18	0.79
1:B:43:LEU:CD1	1:B:69[B]:ILE:CD1	2.64	0.74
1:E:146:ASP:OD1	5:E:2127:HOH:O	2.06	0.74
1:G:57[B]:ILE:CD1	1:I:57[B]:ILE:CD1	2.66	0.73
1:E:57[A]:ILE:HD11	1:L:57[A]:ILE:CD1	2.13	0.73
1:H:72[B]:TYR:HH	1:H:154[B]:SER:HG	0.76	0.72
1:D:57:ILE:HD11	1:G:57[B]:ILE:HD12	1.72	0.71
1:I:152[B]:LYS:CE	5:I:2150:HOH:O	2.37	0.71
1:B:57[B]:ILE:CD1	1:F:57[B]:ILE:CD1	2.65	0.71
1:D:57:ILE:HD11	1:G:57[B]:ILE:HD11	1.72	0.70
1:G:57[B]:ILE:CG1	1:I:57[B]:ILE:CD1	2.68	0.70
1:E:24:ASP:HB2	1:E:139:GLU:OE2	1.92	0.70
1:F:146:ASP:OD1	5:F:2160:HOH:O	2.09	0.70
1:H:56[B]:MET:CE	5:H:2039:HOH:O	2.41	0.68
1:D:117:ARG:HD2	5:D:2137:HOH:O	1.93	0.68
1:G:57[B]:ILE:HG12	1:I:57[B]:ILE:CD1	2.24	0.68
1:F:72[B]:TYR:OH	1:F:154[B]:SER:HB3	1.93	0.67
1:H:146:ASP:OD1	5:H:2161:HOH:O	2.11	0.67
1:G:57[B]:ILE:HD11	1:I:57[B]:ILE:HD11	1.77	0.66
1:H:75[B]:GLU:OE2	5:H:2076:HOH:O	2.14	0.66
1:J:168[B]:GLN:OE1	5:J:2173:HOH:O	2.13	0.65
1:G:57[B]:ILE:CD1	1:I:57[B]:ILE:HD11	2.26	0.65
1:A:57[B]:ILE:HG12	1:H:57[B]:ILE:HD13	1.77	0.65
1:B:146[A]:ASP:OD2	5:B:2151:HOH:O	2.14	0.65
1:H:56[B]:MET:HE1	5:H:2039:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163[B]:GLN:OE1	1:A:170:PRO:O	2.18	0.62
1:A:57[B]:ILE:CG1	1:H:57[B]:ILE:CD1	2.68	0.61
1:F:72[B]:TYR:HE1	5:F:2031:HOH:O	1.84	0.61
1:A:163[B]:GLN:OE1	1:A:170:PRO:HA	2.00	0.61
1:H:57[B]:ILE:HD12	2:K:3173[B]:EPE:O1S	2.01	0.61
1:C:68:GLU:OE2	1:C:72[B]:TYR:OH	2.17	0.61
1:I:40:HIS:CE1	1:I:66[B]:MET:CE	2.83	0.61
1:H:61[B]:LYS:CE	5:H:2050:HOH:O	2.48	0.60
1:F:22:LEU:HB3	1:F:28:VAL:HG22	1.84	0.60
1:A:123:ARG:HH22	1:A:163[B]:GLN:NE2	2.01	0.59
1:E:72[B]:TYR:HE2	1:E:155:ILE:HD11	1.68	0.58
1:A:57[B]:ILE:HD11	1:H:57[B]:ILE:HG12	1.86	0.58
1:D:40:HIS:CD2	1:D:70:ASP:OD2	2.57	0.58
1:A:152[B]:LYS:CE	5:A:2136:HOH:O	2.51	0.57
1:G:72[B]:TYR:HE2	1:G:155:ILE:HD11	1.70	0.57
1:J:40[A]:HIS:CD2	1:J:70:ASP:OD2	2.58	0.57
1:L:24:ASP:HB3	1:L:135:VAL:CG1	2.35	0.57
1:E:68:GLU:OE2	1:E:72[B]:TYR:OH	2.19	0.56
1:G:57[B]:ILE:HG12	1:I:57[B]:ILE:HD11	1.84	0.56
1:G:57[B]:ILE:HG13	1:I:57[B]:ILE:HD11	1.87	0.56
1:L:24:ASP:HB3	1:L:135:VAL:HG11	1.87	0.55
1:B:24:ASP:HB3	1:B:135:VAL:CG1	2.37	0.55
1:B:72:TYR:OH	1:B:154[B]:SER:OG	2.15	0.55
1:G:57[B]:ILE:HG12	1:I:57[B]:ILE:HD13	1.89	0.54
1:I:68:GLU:OE2	1:I:72[B]:TYR:OH	2.23	0.54
1:A:114:GLN:HG3	5:A:2120:HOH:O	2.08	0.54
1:I:152[B]:LYS:HE2	5:I:2150:HOH:O	2.02	0.53
1:E:53:ARG:HB3	2:E:3173[B]:EPE:H61	1.90	0.53
1:B:24:ASP:HB3	1:B:135:VAL:HG11	1.91	0.53
1:F:22:LEU:HD11	1:F:31:GLN:HG2	1.92	0.52
1:B:43:LEU:HD11	1:B:69[B]:ILE:HD12	1.79	0.52
1:E:24:ASP:CB	1:E:139:GLU:OE2	2.57	0.52
1:B:43:LEU:HD12	1:B:69[B]:ILE:CD1	2.38	0.51
1:B:28[B]:VAL:HG11	1:B:132:GLY:HA2	1.93	0.51
1:A:57[B]:ILE:HG13	1:H:57[B]:ILE:HD11	1.90	0.51
1:L:72[B]:TYR:HE2	1:L:155:ILE:HD11	1.76	0.50
1:K:152:LYS:HE3	5:K:2139:HOH:O	2.12	0.50
1:I:130:GLN:OE1	1:I:152[B]:LYS:HE3	2.11	0.50
1:A:57[A]:ILE:HD12	5:A:2022:HOH:O	2.11	0.50
1:H:57[A]:ILE:HD12	5:H:2016:HOH:O	2.13	0.49
1:A:123:ARG:NH2	1:A:163[B]:GLN:NE2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72[B]:TYR:HE1	5:H:2078:HOH:O	1.95	0.48
1:F:28:VAL:HG21	1:F:135[B]:VAL:HG11	1.96	0.48
1:A:114:GLN:NE2	5:A:2127:HOH:O	2.36	0.48
1:D:134:ASP:O	1:D:139:GLU:OE2	2.31	0.48
1:H:72[B]:TYR:OH	1:H:154[B]:SER:OG	1.86	0.48
1:A:57[B]:ILE:CD1	1:H:57[B]:ILE:HD11	2.44	0.47
1:C:57[A]:ILE:HG23	1:C:58:TRP:CD1	2.49	0.47
1:B:43:LEU:HD12	1:B:69[B]:ILE:HD12	1.96	0.47
1:B:152[B]:LYS:CE	5:B:2155:HOH:O	2.58	0.47
1:D:137:ASP:OD1	1:D:139:GLU:OE2	2.33	0.47
1:L:68:GLU:OE2	1:L:72[B]:TYR:OH	2.23	0.47
1:J:138[B]:GLU:HG3	5:J:2149:HOH:O	2.14	0.47
1:B:40:HIS:CD2	1:B:70:ASP:OD2	2.69	0.46
1:C:146:ASP:OD1	5:C:2152:HOH:O	2.20	0.46
1:C:57[B]:ILE:HD11	1:C:58:TRP:CE2	2.50	0.46
1:F:134:ASP:OD1	5:F:2147:HOH:O	2.21	0.46
1:A:130:GLN:OE1	1:A:152[B]:LYS:HE2	2.15	0.46
1:B:57[B]:ILE:CD1	1:J:57[B]:ILE:CD1	2.61	0.45
1:K:63[B]:ASP:HA	1:K:66:MET:HE3	1.98	0.45
1:B:72:TYR:HH	1:B:154[A]:SER:HB3	1.80	0.45
1:G:68:GLU:OE2	1:G:72[B]:TYR:OH	2.22	0.45
1:C:40:HIS:CD2	1:C:70:ASP:OD2	2.70	0.44
2:B:3173[A]:EPE:H61	1:J:53:ARG:HB3	1.98	0.44
1:H:28[B]:VAL:HG11	1:H:132:GLY:CA	2.48	0.44
1:B:28[B]:VAL:HG11	1:B:132:GLY:CA	2.48	0.44
1:B:130:GLN:OE1	1:B:152[B]:LYS:HE3	2.18	0.44
1:H:28[B]:VAL:HG11	1:H:132:GLY:HA2	1.99	0.44
1:A:57[B]:ILE:HD11	1:H:57[B]:ILE:CG1	2.47	0.44
1:B:57[A]:ILE:HD11	1:J:56[A]:MET:HG3	2.00	0.43
1:A:57[B]:ILE:CD1	1:H:57[B]:ILE:CD1	2.95	0.43
1:A:57[B]:ILE:HD11	1:H:57[B]:ILE:CD1	2.48	0.43
1:K:63[A]:ASP:HA	1:K:66:MET:HE3	2.00	0.43
1:A:109:VAL:HG12	1:A:114:GLN:HG2	2.01	0.43
1:L:28[B]:VAL:HG11	1:L:132:GLY:HA2	2.01	0.43
1:D:172:LEU:HD23	1:D:172:LEU:HA	1.86	0.42
1:F:46:VAL:HG13	1:F:114:GLN:HB3	2.01	0.42
1:B:172:LEU:HD11	1:L:82:THR:HG22	2.01	0.41
1:G:146[A]:ASP:OD2	5:G:2130:HOH:O	2.22	0.41
1:L:24:ASP:HB2	1:L:139:GLU:OE2	2.19	0.41
1:L:47:HIS:CE1	1:L:59:HIS:CE1	3.08	0.41
1:A:72:TYR:OH	1:A:154[B]:SER:OG	2.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72[B]:TYR:CE2	1:E:155:ILE:HD11	2.52	0.41
1:G:47:HIS:CE1	1:G:59:HIS:CE1	3.09	0.41
1:K:152:LYS:CE	5:K:2139:HOH:O	2.68	0.41
1:L:28[B]:VAL:HG11	1:L:132:GLY:CA	2.51	0.41
1:D:47:HIS:CE1	1:D:59:HIS:CE1	3.10	0.40
1:I:47:HIS:CE1	1:I:59:HIS:CE1	3.10	0.40
1:D:57:ILE:HA	1:D:57:ILE:HD13	1.85	0.40
1:L:32:ALA:HA	1:L:128:LEU:HD21	2.04	0.40
1:C:57[B]:ILE:HD13	1:L:56[B]:MET:HB3	2.03	0.40
1:D:28[B]:VAL:HG21	1:D:132:GLY:HA2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:OD1	1:B:108:ASN:CB[2_574]	1.95	0.25

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	161/165 (98%)	160 (99%)	1 (1%)	0	100	100
1	B	159/165 (96%)	158 (99%)	1 (1%)	0	100	100
1	C	160/165 (97%)	159 (99%)	1 (1%)	0	100	100
1	D	156/165 (94%)	153 (98%)	2 (1%)	1 (1%)	21	6
1	E	159/165 (96%)	158 (99%)	1 (1%)	0	100	100
1	F	159/165 (96%)	157 (99%)	2 (1%)	0	100	100
1	G	158/165 (96%)	157 (99%)	1 (1%)	0	100	100
1	H	164/165 (99%)	163 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	160/165 (97%)	159 (99%)	1 (1%)	0	100	100
1	J	160/165 (97%)	159 (99%)	1 (1%)	0	100	100
1	K	155/165 (94%)	153 (99%)	2 (1%)	0	100	100
1	L	157/165 (95%)	156 (99%)	1 (1%)	0	100	100
All	All	1908/1980 (96%)	1892 (99%)	15 (1%)	1 (0%)	48	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	139	GLU

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	138/139 (99%)	136 (99%)	2 (1%)	59	33
1	B	133/139 (96%)	130 (98%)	3 (2%)	44	16
1	C	135/139 (97%)	135 (100%)	0	100	100
1	D	131/139 (94%)	127 (97%)	4 (3%)	35	9
1	E	134/139 (96%)	134 (100%)	0	100	100
1	F	135/139 (97%)	135 (100%)	0	100	100
1	G	133/139 (96%)	133 (100%)	0	100	100
1	H	142/139 (102%)	142 (100%)	0	100	100
1	I	134/139 (96%)	131 (98%)	3 (2%)	45	17
1	J	134/139 (96%)	133 (99%)	1 (1%)	76	57
1	K	132/139 (95%)	132 (100%)	0	100	100
1	L	132/139 (95%)	131 (99%)	1 (1%)	73	54
All	All	1613/1668 (97%)	1599 (99%)	14 (1%)	73	49

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99[A]	GLN
1	A	99[B]	GLN
1	B	44	HIS
1	B	117[A]	ARG
1	B	117[B]	ARG
1	D	44	HIS
1	D	69	ILE
1	D	104	LEU
1	D	139	GLU
1	I	44	HIS
1	I	69	ILE
1	I	117	ARG
1	J	44	HIS
1	L	44	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	D	130	GLN
1	E	45	GLN
1	E	108	ASN
1	F	45	GLN
1	G	45	GLN
1	H	45	GLN
1	I	45	GLN
1	L	45	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

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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
2	EPE	K	3173[B]	-	15,15,15	0.87	1 (6%)	19,20,20	2.02	5 (26%)
2	EPE	B	3173[A]	-	15,15,15	0.78	1 (6%)	19,20,20	2.14	4 (21%)
2	EPE	G	3173	-	15,15,15	0.67	1 (6%)	19,20,20	1.49	3 (15%)
2	EPE	E	3173[A]	-	15,15,15	0.99	1 (6%)	19,20,20	2.12	5 (26%)
2	EPE	K	3173[A]	-	15,15,15	0.80	1 (6%)	19,20,20	2.16	7 (36%)
2	EPE	E	3173[B]	-	15,15,15	0.74	1 (6%)	19,20,20	1.95	3 (15%)
2	EPE	B	3173[B]	-	15,15,15	0.73	1 (6%)	19,20,20	1.76	5 (26%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	K	3173[B]	-	-	4/9/19/19	0/1/1/1
2	EPE	B	3173[A]	-	-	6/9/19/19	0/1/1/1
2	EPE	G	3173	-	-	2/9/19/19	0/1/1/1
2	EPE	E	3173[A]	-	-	4/9/19/19	0/1/1/1
2	EPE	K	3173[A]	-	-	5/9/19/19	0/1/1/1
2	EPE	E	3173[B]	-	-	2/9/19/19	0/1/1/1
2	EPE	B	3173[B]	-	-	4/9/19/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3173[A]	EPE	C10-S	3.47	1.82	1.77
2	K	3173[B]	EPE	C10-S	3.04	1.81	1.77
2	B	3173[A]	EPE	C10-S	2.76	1.81	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	3173[A]	EPE	C10-S	2.53	1.81	1.77
2	E	3173[B]	EPE	C10-S	2.44	1.81	1.77
2	B	3173[B]	EPE	C10-S	2.17	1.80	1.77
2	G	3173	EPE	C10-S	2.11	1.80	1.77

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3173[B]	EPE	C5-N4-C3	6.49	122.82	108.84
2	E	3173[A]	EPE	C5-N4-C3	6.04	121.85	108.84
2	K	3173[B]	EPE	C5-N4-C3	5.68	121.07	108.84
2	B	3173[A]	EPE	O1S-S-C10	5.50	115.03	106.73
2	K	3173[A]	EPE	O1S-S-C10	5.04	114.34	106.73
2	B	3173[A]	EPE	C5-N4-C3	4.80	119.17	108.84
2	B	3173[B]	EPE	C5-N4-C3	4.51	118.56	108.84
2	E	3173[A]	EPE	O1S-S-C10	4.23	113.11	106.73
2	K	3173[A]	EPE	C6-N1-C2	3.87	117.17	108.84
2	K	3173[A]	EPE	C5-N4-C3	3.38	116.12	108.84
2	K	3173[A]	EPE	C7-N4-C3	3.23	119.83	111.24
2	K	3173[B]	EPE	O2S-S-C10	3.17	111.51	106.73
2	B	3173[A]	EPE	O2S-S-C10	-3.15	101.97	106.73
2	B	3173[B]	EPE	O2S-S-C10	3.00	111.27	106.73
2	E	3173[A]	EPE	C7-N4-C3	2.92	119.02	111.24
2	B	3173[B]	EPE	C7-N4-C5	2.88	118.92	111.24
2	B	3173[B]	EPE	O1S-S-C10	-2.81	102.48	106.73
2	B	3173[B]	EPE	C7-N4-C3	2.81	118.72	111.24
2	E	3173[A]	EPE	C7-N4-C5	2.77	118.62	111.24
2	K	3173[B]	EPE	O3S-S-C10	2.66	111.21	106.00
2	E	3173[B]	EPE	C6-C5-N4	2.61	115.92	110.65
2	B	3173[A]	EPE	C7-N4-C3	2.38	117.59	111.24
2	G	3173	EPE	C5-N4-C3	2.36	113.92	108.84
2	K	3173[A]	EPE	C7-N4-C5	2.31	117.39	111.24
2	G	3173	EPE	C3-C2-N1	-2.28	106.05	110.65
2	E	3173[A]	EPE	C9-N1-C2	2.23	117.18	111.24
2	K	3173[A]	EPE	C9-N1-C6	-2.19	105.40	111.24
2	K	3173[A]	EPE	O2S-S-C10	-2.18	103.44	106.73
2	K	3173[B]	EPE	C7-N4-C3	2.16	117.00	111.24
2	K	3173[B]	EPE	C2-C3-N4	2.15	114.99	110.65
2	G	3173	EPE	C10-C9-N1	-2.08	104.48	112.36
2	E	3173[B]	EPE	C2-C3-N4	2.07	114.82	110.65

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3173[A]	EPE	C9-C10-S-O2S
2	B	3173[B]	EPE	C10-C9-N1-C2
2	B	3173[B]	EPE	C10-C9-N1-C6
2	K	3173[A]	EPE	C9-C10-S-O1S
2	K	3173[A]	EPE	C9-C10-S-O2S
2	K	3173[B]	EPE	C10-C9-N1-C6
2	B	3173[A]	EPE	N4-C7-C8-O8
2	E	3173[A]	EPE	C9-C10-S-O3S
2	B	3173[A]	EPE	C9-C10-S-O3S
2	K	3173[A]	EPE	C9-C10-S-O3S
2	E	3173[B]	EPE	N4-C7-C8-O8
2	B	3173[A]	EPE	C10-C9-N1-C2
2	G	3173	EPE	C10-C9-N1-C2
2	K	3173[B]	EPE	C10-C9-N1-C2
2	E	3173[A]	EPE	C8-C7-N4-C5
2	K	3173[A]	EPE	C8-C7-N4-C5
2	B	3173[A]	EPE	C9-C10-S-O1S
2	E	3173[A]	EPE	C9-C10-S-O1S
2	E	3173[A]	EPE	C9-C10-S-O2S
2	B	3173[A]	EPE	C10-C9-N1-C6
2	K	3173[B]	EPE	C8-C7-N4-C3
2	B	3173[B]	EPE	C8-C7-N4-C3
2	K	3173[A]	EPE	C8-C7-N4-C3
2	G	3173	EPE	C10-C9-N1-C6
2	K	3173[B]	EPE	N4-C7-C8-O8
2	B	3173[B]	EPE	C8-C7-N4-C5
2	E	3173[B]	EPE	C8-C7-N4-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	3173[B]	EPE	1	0
2	B	3173[A]	EPE	1	0
2	E	3173[B]	EPE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	156/165 (94%)	-0.14	9 (5%) 29 31	7, 14, 27, 35	9 (5%)
1	B	150/165 (90%)	-0.28	3 (2%) 65 68	9, 15, 25, 30	11 (7%)
1	C	152/165 (92%)	-0.31	2 (1%) 75 78	8, 14, 24, 37	10 (6%)
1	D	152/165 (92%)	-0.32	0 100 100	9, 14, 22, 29	6 (3%)
1	E	151/165 (91%)	-0.28	1 (0%) 84 87	9, 15, 23, 35	10 (6%)
1	F	151/165 (91%)	-0.46	0 100 100	7, 13, 21, 28	10 (6%)
1	G	153/165 (92%)	-0.31	0 100 100	8, 16, 24, 40	7 (4%)
1	H	151/165 (91%)	-0.40	3 (1%) 65 68	7, 13, 21, 32	15 (9%)
1	I	152/165 (92%)	-0.41	3 (1%) 65 68	8, 14, 22, 35	10 (6%)
1	J	151/165 (91%)	-0.55	1 (0%) 84 87	7, 13, 20, 25	11 (7%)
1	K	151/165 (91%)	-0.45	3 (1%) 65 68	8, 13, 20, 28	6 (3%)
1	L	151/165 (91%)	-0.29	2 (1%) 75 78	8, 15, 25, 34	8 (5%)
All	All	1821/1980 (91%)	-0.35	27 (1%) 72 75	7, 14, 23, 40	113 (6%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	23	ALA	5.5
1	A	14	ALA	4.9
1	A	17	SER	4.7
1	L	22	LEU	4.5
1	A	16	PHE	4.2
1	C	22	LEU	3.8
1	A	18	PRO	3.5
1	B	172	LEU	3.4
1	K	172	LEU	3.3
1	K	22	LEU	3.3
1	A	172	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	22	LEU	3.2
1	A	20	PRO	3.2
1	I	172	LEU	3.2
1	A	108	ASN	3.1
1	I	21	SER	3.0
1	K	23	ALA	3.0
1	J	172	LEU	2.9
1	A	15	SER	2.9
1	A	109	VAL	2.8
1	H	22	LEU	2.8
1	C	172	LEU	2.3
1	H	172	LEU	2.2
1	L	23	ALA	2.1
1	B	108	ASN	2.1
1	B	23	ALA	2.1
1	I	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(Å ²)	Q<0.9
2	EPE	E	3173[A]	15/15	0.94	0.11	18,21,28,31	15
2	EPE	E	3173[B]	15/15	0.94	0.11	17,22,28,31	15
2	EPE	B	3173[A]	15/15	0.95	0.09	24,29,33,34	15
2	EPE	B	3173[B]	15/15	0.95	0.09	13,19,25,25	15
2	EPE	K	3173[A]	15/15	0.95	0.10	19,24,32,34	15
2	EPE	K	3173[B]	15/15	0.95	0.10	16,24,28,28	15
2	EPE	G	3173	15/15	0.96	0.08	17,20,28,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	CA	D	3173	1/1	0.98	0.05	18,18,18,18	1
4	CL	J	3173	1/1	0.99	0.03	14,14,14,14	0
4	CL	K	3174	1/1	0.99	0.04	16,16,16,16	0
3	CA	J	3174	1/1	1.00	0.02	11,11,11,11	0
3	CA	K	3175	1/1	1.00	0.03	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.