



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:39 am GMT

PDB ID : 2CF7
Title : ASP74ALA MUTANT CRYSTAL STRUCTURE FOR DPS-LIKE PEROX-
IDE 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

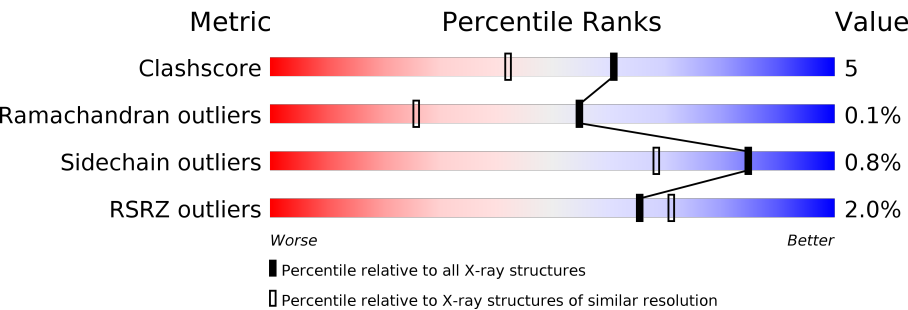
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	<div><div>5%</div><div>87%7%5%</div></div>
1	B	165	<div><div>2%</div><div>79%12%9%</div></div>
1	C	165	<div><div>2%</div><div>89%8%</div></div>
1	D	165	<div><div>%</div><div>83%8%8%</div></div>
1	E	165	<div><div>%</div><div>87%8%</div></div>
1	F	165	<div><div>%</div><div>83%8%8%</div></div>
1	G	165	<div><div>2%</div><div>87%5%7%</div></div>

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Mol	Chain	Length	Quality of chain
1	H	165	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>85%</div><div>7%</div><div>8%</div></div></div>
1	I	165	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>87%</div><div>5%</div><div>8%</div></div></div>
1	J	165	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>86%</div><div>5%</div><div>8%</div></div></div>
1	K	165	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>90%</div><div></div><div>8%</div></div></div>
1	L	165	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>82%</div><div>9%</div><div>8%</div></div></div>

2 Entry composition

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

There are 12 discrepancies between the modelled and reference sequences:

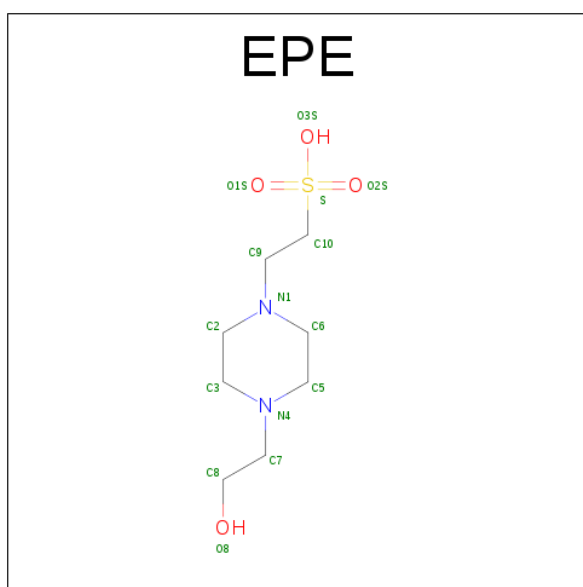
Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	ASP	ENGINEERED MUTATION	UNP Q9F5J9
B	74	ALA	ASP	ENGINEERED MUTATION	UNP Q9F5J9
C	74	ALA	ASP	ENGINEERED MUTATION	UNP Q9F5J9
D	74	ALA	ASP	ENGINEERED MUTATION	UNP Q9F5J9
E	74	ALA	ASP	ENGINEERED MUTATION	UNP Q9F5J9

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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 (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (three-letter code: CA) (formula: Ca).

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

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

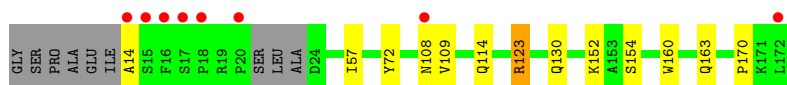
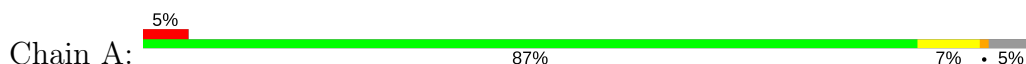
- Molecule 5 is water.

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

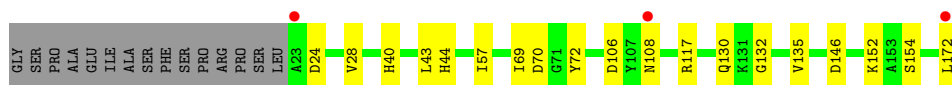
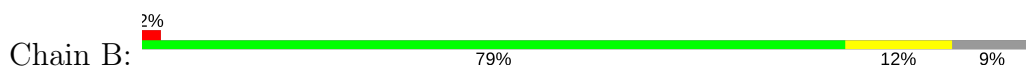
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

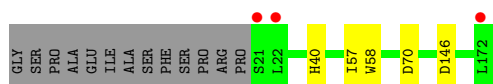
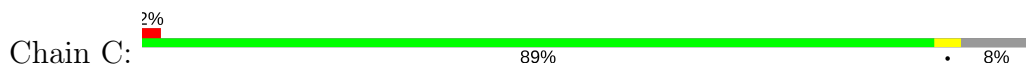
• Molecule 1: DPR



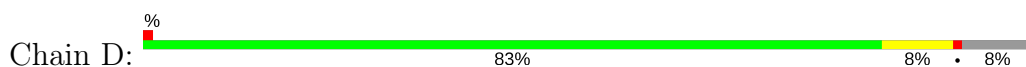
• Molecule 1: DPR



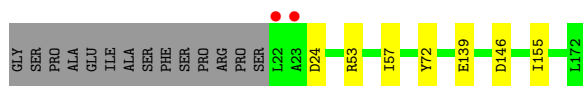
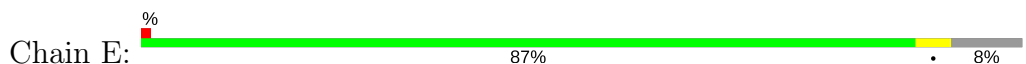
• Molecule 1: DPR



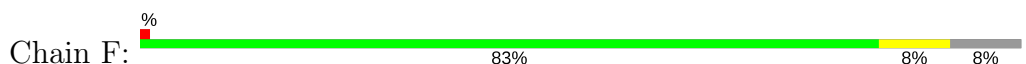
• Molecule 1: DPR



• Molecule 1: DPR

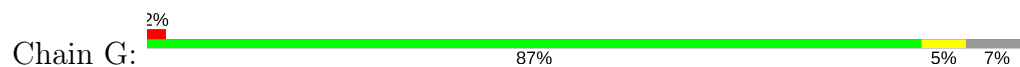


• Molecule 1: DPR

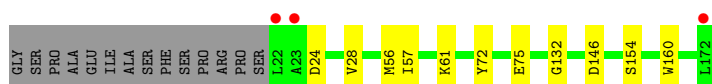
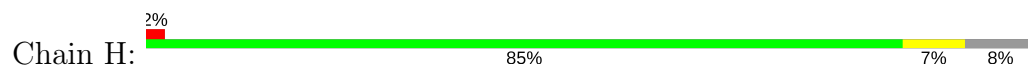




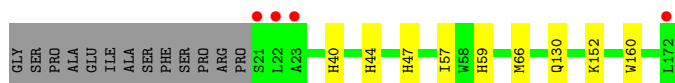
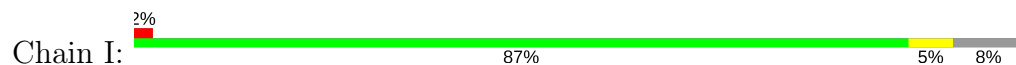
• Molecule 1: DPR



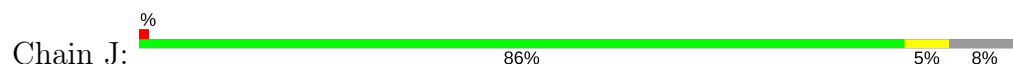
• Molecule 1: DPR



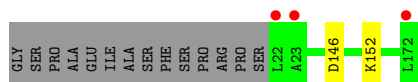
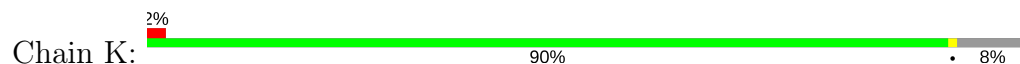
• Molecule 1: DPR



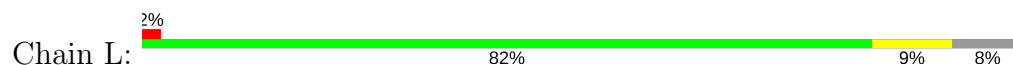
• Molecule 1: DPR



• Molecule 1: DPR



• Molecule 1: DPR



4 Data and refinement statistics

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) 100.0 (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)	Xtriage
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.	DCC
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
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

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EPE, 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	0.70	0/1328	0.77	2/1795 (0.1%)
1	B	0.66	0/1296	0.72	0/1750
1	C	0.66	0/1302	0.75	0/1761
1	D	0.77	2/1270 (0.2%)	0.77	0/1718
1	E	0.62	0/1301	0.71	0/1760
1	F	0.71	0/1303	0.77	1/1763 (0.1%)
1	G	0.64	0/1287	0.76	1/1741 (0.1%)
1	H	0.69	0/1352	0.81	1/1826 (0.1%)
1	I	0.66	0/1305	0.72	0/1765
1	J	0.69	0/1305	0.77	0/1763
1	K	0.74	0/1271	0.80	0/1717
1	L	0.63	0/1281	0.74	0/1732
All	All	0.68	2/15601 (0.0%)	0.76	5/21091 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	139	GLU	CB-CG	9.69	1.70	1.52
1	D	139	GLU	CD-OE2	6.87	1.33	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	H	24	ASP	CB-CG-OD1	6.08	123.77	118.30
1	G	20	PRO	N-CA-CB	5.83	110.29	103.30
1	F	129	PHE	CB-CG-CD1	-5.36	117.05	120.80
1	A	123	ARG	NE-CZ-NH2	-5.35	117.62	120.30

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

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	5	0
1	D	1227	0	1197	11	0
1	E	1245	0	1225	8	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	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	179	0	0	4	0
5	C	170	0	0	1	0
5	D	183	0	0	1	0
5	E	153	0	0	1	0
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	155	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 (155) 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:F:57[B]:ILE:CD1	1:J:57[B]:ILE:CD1	2.33	1.05
1:B:57[B]:ILE:HD11	1:J:57[B]:ILE:HD11	1.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:57[B]:ILE:HD11	1:F:57[B]:ILE:CD1	2.09	0.79
1:B:43:LEU:HD11	1:B:69[B]:ILE:CD1	2.13	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	0.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:I:40:HIS:CE1	1:I:66[B]:MET:HE3	2.36	0.60
1:B:72:TYR:OH	1:B:154[B]:SER:OG	2.15	0.59
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: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:A:72:TYR:OH	1:A:154[B]:SER:OG	2.13	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:G:57[B]:ILE:HG12	1:I:57[B]:ILE:HD13	1.89	0.54
1:H:56[B]:MET:HE3	5:H:2039:HOH:O	2.04	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:152[B]:LYS:NZ	5:B:2155:HOH:O	2.16	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:57[A]:ILE:HG23	1:C:58:TRP:CD1	2.49	0.47
1:A:57[B]:ILE:CD1	1:H:57[B]:ILE:HD11	2.44	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:I:40:HIS:CE1	1:I:66[B]:MET:HE2	2.49	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: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: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

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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:HD13	1:D:57:ILE:HA	1.85	0.40
1:L:32:ALA:HA	1:L:128:LEU:HD21	2.04	0.40
1:D:28[B]:VAL:HG21	1:D:132:GLY:HA2	2.04	0.40
1:C:57[B]:ILE:HD13	1:L:56[B]:MET:HB3	2.03	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

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	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%)	28	7
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%)	55	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	139	GLU

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	138/139 (99%)	137 (99%)	1 (1%)	87	72
1	B	133/139 (96%)	130 (98%)	3 (2%)	56	23
1	C	135/139 (97%)	135 (100%)	0	100	100
1	D	131/139 (94%)	128 (98%)	3 (2%)	56	23
1	E	134/139 (96%)	134 (100%)	0	100	100
1	F	135/139 (97%)	134 (99%)	1 (1%)	87	72
1	G	133/139 (96%)	132 (99%)	1 (1%)	85	68
1	H	142/139 (102%)	141 (99%)	1 (1%)	87	72
1	I	134/139 (96%)	132 (98%)	2 (2%)	70	42
1	J	134/139 (96%)	133 (99%)	1 (1%)	87	72
1	K	132/139 (95%)	132 (100%)	0	100	100
1	L	132/139 (95%)	132 (100%)	0	100	100
All	All	1613/1668 (97%)	1600 (99%)	13 (1%)	85	68

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	TRP
1	B	44	HIS
1	B	117[A]	ARG
1	B	117[B]	ARG
1	D	44	HIS
1	D	104	LEU
1	D	139	GLU
1	F	44	HIS
1	G	160	TRP
1	H	160	TRP
1	I	44	HIS
1	I	160	TRP
1	J	44	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	108	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	B	3173[A]	-	15,15,15	0.76	1 (6%)	18,20,20	3.09	5 (27%)
2	EPE	B	3173[B]	-	15,15,15	0.72	1 (6%)	18,20,20	2.29	5 (27%)
2	EPE	E	3173[A]	-	15,15,15	0.96	1 (6%)	18,20,20	2.58	5 (27%)
2	EPE	E	3173[B]	-	15,15,15	0.73	1 (6%)	18,20,20	2.13	5 (27%)
2	EPE	G	3173	-	15,15,15	0.66	1 (6%)	18,20,20	1.72	5 (27%)
2	EPE	K	3173[A]	-	15,15,15	0.79	1 (6%)	18,20,20	2.87	7 (38%)
2	EPE	K	3173[B]	-	15,15,15	0.84	1 (6%)	18,20,20	2.42	5 (27%)

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
2	EPE	B	3173[A]	-	-	0/9/19/19	0/1/1/1
2	EPE	B	3173[B]	-	-	0/9/19/19	0/1/1/1
2	EPE	E	3173[A]	-	-	0/9/19/19	0/1/1/1
2	EPE	E	3173[B]	-	-	0/9/19/19	0/1/1/1
2	EPE	G	3173	-	-	0/9/19/19	0/1/1/1
2	EPE	K	3173[A]	-	-	0/9/19/19	0/1/1/1
2	EPE	K	3173[B]	-	-	0/9/19/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3173	EPE	C10-S	2.07	1.80	1.77
2	B	3173[B]	EPE	C10-S	2.12	1.80	1.77
2	E	3173[B]	EPE	C10-S	2.38	1.81	1.77
2	K	3173[A]	EPE	C10-S	2.46	1.81	1.77
2	B	3173[A]	EPE	C10-S	2.67	1.81	1.77
2	K	3173[B]	EPE	C10-S	2.94	1.81	1.77
2	E	3173[A]	EPE	C10-S	3.34	1.82	1.77

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3173[A]	EPE	O2S-S-C10	-5.61	101.97	106.79
2	B	3173[B]	EPE	O1S-S-C10	-5.02	102.48	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3173[A]	EPE	O2S-S-C10	-3.91	103.44	106.79
2	E	3173[B]	EPE	O3S-S-C10	-3.16	102.17	106.06
2	K	3173[A]	EPE	C9-N1-C6	-2.28	105.40	111.26
2	G	3173	EPE	C3-C2-N1	-2.27	106.05	110.63
2	E	3173[B]	EPE	C2-C3-N4	2.07	114.82	110.63
2	G	3173	EPE	O3S-S-O2S	2.07	116.12	111.37
2	K	3173[B]	EPE	C2-C3-N4	2.15	114.99	110.63
2	G	3173	EPE	C5-N4-C3	2.23	113.92	108.87
2	K	3173[B]	EPE	C7-N4-C3	2.24	117.00	111.26
2	E	3173[A]	EPE	C9-N1-C2	2.31	117.18	111.26
2	K	3173[A]	EPE	C7-N4-C5	2.39	117.39	111.26
2	B	3173[A]	EPE	C7-N4-C3	2.47	117.59	111.26
2	E	3173[B]	EPE	C6-C5-N4	2.61	115.92	110.63
2	E	3173[A]	EPE	C7-N4-C5	2.87	118.62	111.26
2	B	3173[B]	EPE	C7-N4-C3	2.91	118.72	111.26
2	B	3173[A]	EPE	O3S-S-C10	2.94	109.67	106.06
2	B	3173[B]	EPE	C7-N4-C5	2.99	118.92	111.26
2	G	3173	EPE	O2S-S-C10	3.03	109.39	106.79
2	E	3173[A]	EPE	C7-N4-C3	3.03	119.02	111.26
2	E	3173[B]	EPE	O2S-S-C10	3.17	109.52	106.79
2	K	3173[A]	EPE	C5-N4-C3	3.20	116.12	108.87
2	K	3173[A]	EPE	C7-N4-C3	3.35	119.83	111.26
2	G	3173	EPE	O1S-S-C10	3.44	109.74	106.79
2	K	3173[A]	EPE	C6-N1-C2	3.66	117.17	108.87
2	K	3173[B]	EPE	O3S-S-C10	4.19	111.21	106.06
2	B	3173[B]	EPE	C5-N4-C3	4.28	118.56	108.87
2	B	3173[A]	EPE	C5-N4-C3	4.55	119.17	108.87
2	B	3173[B]	EPE	O2S-S-C10	5.21	111.27	106.79
2	K	3173[B]	EPE	C5-N4-C3	5.39	121.07	108.87
2	K	3173[B]	EPE	O2S-S-C10	5.50	111.51	106.79
2	E	3173[A]	EPE	C5-N4-C3	5.73	121.85	108.87
2	E	3173[B]	EPE	C5-N4-C3	6.16	122.82	108.87
2	E	3173[A]	EPE	O1S-S-C10	7.36	113.11	106.79
2	K	3173[A]	EPE	O1S-S-C10	8.79	114.34	106.79
2	B	3173[A]	EPE	O1S-S-C10	9.60	115.03	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3173[A]	EPE	1	0
2	E	3173[B]	EPE	1	0
2	K	3173[B]	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(Å²)	Q<0.9
1	A	156/165 (94%)	-0.16	8 (5%)	29	32	10, 15, 27, 35	0
1	B	150/165 (90%)	-0.32	3 (2%)	65	71	11, 16, 25, 30	0
1	C	152/165 (92%)	-0.31	3 (1%)	65	71	12, 15, 24, 37	0
1	D	152/165 (92%)	-0.37	1 (0%)	87	90	12, 15, 22, 29	0
1	E	151/165 (91%)	-0.31	2 (1%)	77	81	13, 16, 23, 35	0
1	F	151/165 (91%)	-0.50	1 (0%)	87	90	11, 13, 21, 28	0
1	G	153/165 (92%)	-0.31	3 (1%)	65	71	13, 16, 24, 40	0
1	H	151/165 (91%)	-0.42	3 (1%)	65	71	10, 13, 21, 32	0
1	I	152/165 (92%)	-0.41	4 (2%)	56	62	12, 14, 22, 35	0
1	J	151/165 (91%)	-0.52	2 (1%)	77	81	10, 13, 21, 25	0
1	K	151/165 (91%)	-0.46	3 (1%)	65	71	10, 13, 21, 28	0
1	L	151/165 (91%)	-0.31	3 (1%)	65	71	13, 15, 25, 34	0
All	All	1821/1980 (91%)	-0.37	36 (1%)	65	71	10, 15, 23, 40	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	22	LEU	8.2
1	A	20	PRO	6.4
1	A	17	SER	5.6
1	H	23	ALA	5.5
1	E	22	LEU	5.3
1	G	20	PRO	5.3
1	K	22	LEU	5.2
1	I	21	SER	5.1
1	C	22	LEU	4.5
1	G	21	SER	4.4
1	A	14	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	K	23	ALA	4.3
1	L	23	ALA	4.2
1	B	172	LEU	4.1
1	A	18	PRO	3.9
1	A	172	LEU	3.8
1	C	21	SER	3.7
1	A	16	PHE	3.4
1	I	22	LEU	3.2
1	I	172	LEU	3.2
1	H	22	LEU	3.1
1	K	172	LEU	3.1
1	H	172	LEU	3.1
1	E	23	ALA	3.1
1	A	108	ASN	3.0
1	C	172	LEU	2.9
1	J	172	LEU	2.9
1	B	23	ALA	2.8
1	L	172	LEU	2.5
1	A	15	SER	2.5
1	F	22	LEU	2.4
1	B	108	ASN	2.4
1	I	23	ALA	2.3
1	J	22	LEU	2.2
1	G	172	LEU	2.1
1	D	172	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	EPE	K	3173[A]	15/15	0.97	0.12	1.87	19,24,32,34	15
2	EPE	K	3173[B]	15/15	0.97	0.12	1.86	16,24,28,28	15
2	EPE	B	3173[A]	15/15	0.98	0.10	1.70	24,29,33,34	15
2	EPE	B	3173[B]	15/15	0.98	0.10	1.69	13,19,25,25	15
3	CA	D	3173	1/1	0.99	0.11	1.11	18,18,18,18	1
2	EPE	E	3173[A]	15/15	0.97	0.11	0.49	18,21,28,31	15
2	EPE	E	3173[B]	15/15	0.97	0.11	0.48	17,22,28,31	15
2	EPE	G	3173	15/15	0.98	0.07	-0.21	17,20,28,32	0
4	CL	K	3174	1/1	0.99	0.03	-2.39	16,16,16,16	0
4	CL	J	3173	1/1	1.00	0.02	-4.72	14,14,14,14	0
3	CA	K	3175	1/1	1.00	0.03	-6.24	11,11,11,11	0
3	CA	J	3174	1/1	1.00	0.02	-8.61	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.