



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:32 AM GMT

PDB ID : 3B62
Title : EmrE multidrug transporter in complex with P4P, P21 crystal form
Authors : Chang, G.; Chen, Y.J.
Deposited on : 2007-10-26
Resolution : 4.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

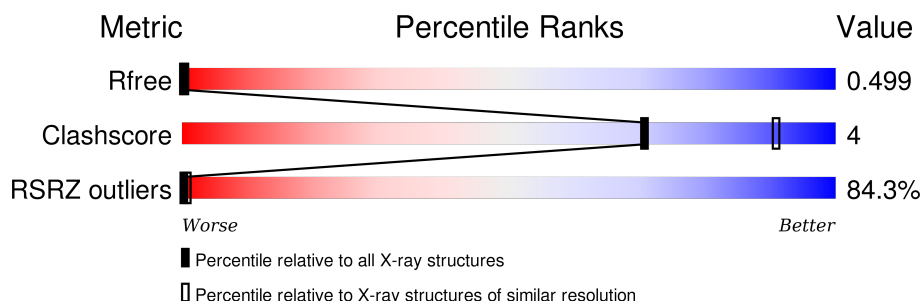
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1067 (5.20-3.60)
Clashscore	102246	1175 (5.20-3.60)
RSRZ outliers	91569	1071 (5.20-3.60)

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	110	 <p>75% (upper red bar), 86% (green), 14% (grey)</p>
1	B	110	 <p>64% (upper red bar), 79% (green), 21% (grey)</p>
1	C	110	 <p>75% (upper red bar), 86% (green), 14% (grey)</p>
1	D	110	 <p>65% (upper red bar), 79% (green), 21% (grey)</p>

2 Entry composition [i](#)

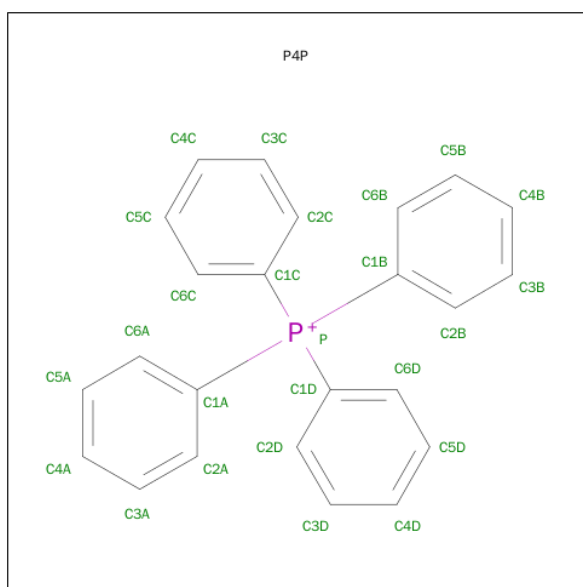
There are 2 unique types of molecules in this entry. The entry contains 414 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Multidrug transporter emrE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	95	Total C 95 95	0	0	95
1	B	87	Total C 87 87	0	0	87
1	C	95	Total C 95 95	0	0	95
1	D	87	Total C 87 87	0	0	87

- Molecule 2 is TETRAPHENYLPHOSPHONIUM (three-letter code: P4P) (formula: $C_{24}H_{20}P$).

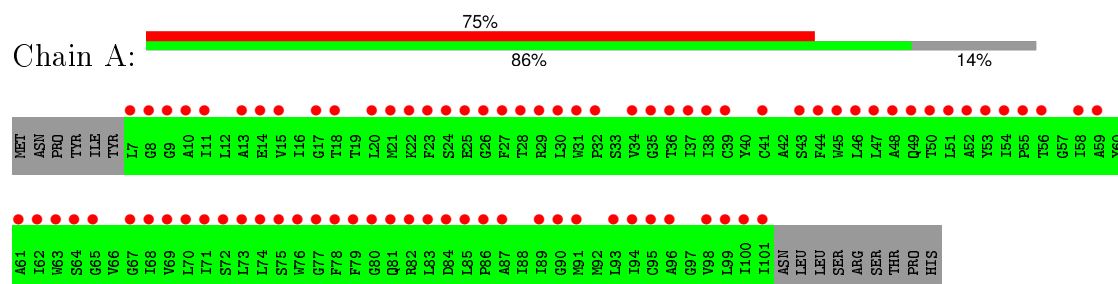


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C P 25 24 1	0	0
2	C	1	Total C P 25 24 1	0	0

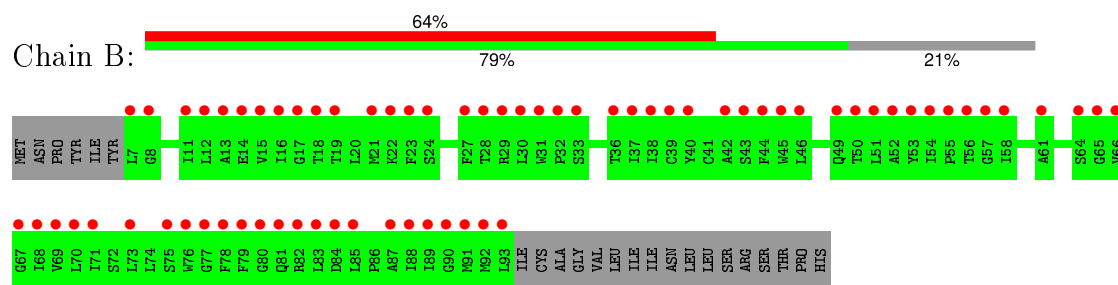
3 Residue-property plots

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

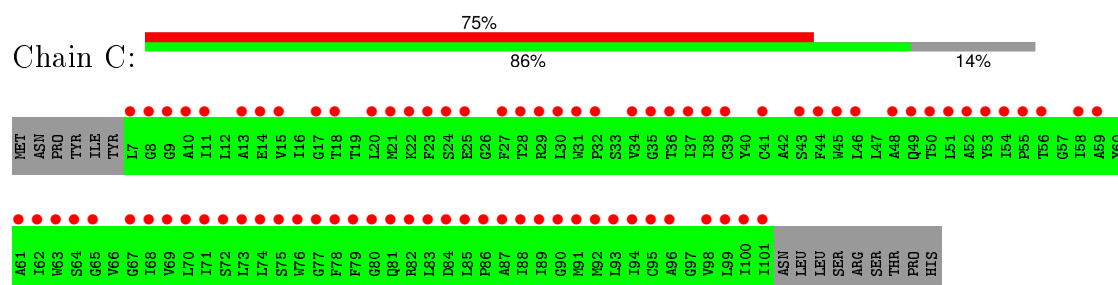
• Molecule 1: Multidrug transporter emrE



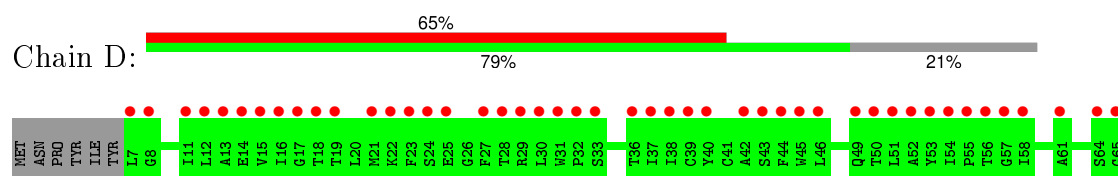
• Molecule 1: Multidrug transporter emrE



• Molecule 1: Multidrug transporter emrE



• Molecule 1: Multidrug transporter emrE



V66	G67	I68	V69	L70	I71	S72	L73	L74	S75	W76	G77	F78	F79	G80	Q81	R82	L83	D84	L85	P86	A87	I88	I89	G90	N91	N92	L93	I94	C95	A96	G97	V98	I99	I100	A101	A102	S103	S104	R105	R106	T107	P108	H109
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.50Å 42.70Å 115.40Å 90.00° 109.10° 90.00°	Depositor
Resolution (Å)	19.80 – 4.40 19.79 – 4.40	Depositor EDS
% Data completeness (in resolution range)	72.9 (19.80-4.40) 72.9 (19.79-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.61 (at 4.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.343 , 0.364 0.533 , 0.499	Depositor DCC
R_{free} test set	345 reflections (11.32%)	DCC
Wilson B-factor (Å ²)	153.5	Xtriage
Anisotropy	0.933	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.07 , 269.2	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 3394 reflections	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	414	wwPDB-VP
Average B, all atoms (Å ²)	178.0	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 94.24 % 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 3.2685e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: P4P

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	95	0	0	0	0
1	B	87	0	0	0	0
1	C	95	0	0	0	0
1	D	87	0	0	0	0
2	A	25	0	20	1	0
2	C	25	0	20	1	0
All	All	414	0	40	2	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 4.

All (2) 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)
2:A:350:P4P:H2C	2:A:350:P4P:C6D	2.49	0.43
2:C:750:P4P:H2C	2:C:750:P4P:C6D	2.49	0.42

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

2 ligands are modelled in this entry.

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	P4P	A	350	-	28,28,28	3.59	22 (78%)	38,38,38	2.02	13 (34%)
2	P4P	C	750	-	28,28,28	3.57	22 (78%)	38,38,38	2.03	14 (36%)

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	P4P	A	350	-	-	0/24/24/24	0/4/4/4
2	P4P	C	750	-	-	0/24/24/24	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	P4P	C3B-C4B	2.06	1.43	1.38
2	C	750	P4P	C3B-C4B	2.06	1.43	1.38
2	A	350	P4P	C6B-C1B	2.07	1.43	1.39
2	C	750	P4P	C3D-C4D	2.07	1.43	1.38
2	C	750	P4P	C6B-C1B	2.13	1.43	1.39
2	A	350	P4P	C3D-C4D	2.17	1.43	1.38
2	A	350	P4P	C5B-C6B	2.20	1.43	1.38
2	C	750	P4P	C5B-C6B	2.21	1.43	1.38
2	C	750	P4P	C2A-C1A	2.42	1.43	1.39
2	A	350	P4P	C2A-C1A	2.59	1.44	1.39
2	C	750	P4P	C4D-C5D	2.76	1.45	1.38
2	A	350	P4P	C4D-C5D	2.89	1.45	1.38
2	A	350	P4P	C5A-C4A	3.05	1.45	1.38
2	C	750	P4P	C5A-C4A	3.06	1.45	1.38
2	C	750	P4P	C4C-C5C	3.17	1.46	1.38
2	C	750	P4P	C3A-C2A	3.17	1.45	1.38
2	C	750	P4P	P-C1C	3.19	1.85	1.79
2	A	350	P4P	C4C-C5C	3.23	1.46	1.38
2	A	350	P4P	C3A-C2A	3.24	1.45	1.38
2	A	350	P4P	P-C1C	3.34	1.85	1.79
2	C	750	P4P	C3C-C4C	3.55	1.47	1.38
2	A	350	P4P	C3C-C4C	3.64	1.47	1.38
2	C	750	P4P	P-C1A	3.77	1.86	1.79
2	C	750	P4P	C6C-C1C	3.81	1.46	1.39
2	A	350	P4P	C6C-C1C	4.01	1.46	1.39
2	A	350	P4P	P-C1A	4.16	1.87	1.79
2	A	350	P4P	P-C1D	4.51	1.88	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	P4P	C3B-C2B	4.54	1.48	1.38
2	C	750	P4P	C5D-C6D	4.55	1.48	1.38
2	C	750	P4P	C3B-C2B	4.61	1.48	1.38
2	C	750	P4P	C2C-C1C	4.64	1.47	1.39
2	A	350	P4P	C2C-C1C	4.67	1.47	1.39
2	A	350	P4P	P-C1B	4.71	1.88	1.79
2	A	350	P4P	C5D-C6D	4.71	1.48	1.38
2	A	350	P4P	C2B-C1B	4.80	1.48	1.39
2	C	750	P4P	P-C1D	4.81	1.88	1.79
2	C	750	P4P	C2B-C1B	4.89	1.48	1.39
2	C	750	P4P	P-C1B	5.10	1.89	1.79
2	C	750	P4P	C2D-C1D	5.34	1.49	1.39
2	A	350	P4P	C2D-C1D	5.39	1.49	1.39
2	C	750	P4P	C5A-C6A	5.75	1.50	1.38
2	A	350	P4P	C5A-C6A	5.81	1.50	1.38
2	C	750	P4P	C6D-C1D	6.05	1.50	1.39
2	A	350	P4P	C6D-C1D	6.16	1.50	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	750	P4P	P-C1C-C2C	-3.71	113.31	120.05
2	A	350	P4P	P-C1C-C2C	-3.71	113.32	120.05
2	A	350	P4P	P-C1B-C2B	-3.19	114.25	120.05
2	C	750	P4P	C4A-C5A-C6A	-3.19	115.51	120.19
2	C	750	P4P	C3A-C2A-C1A	-3.16	116.00	120.29
2	C	750	P4P	P-C1B-C2B	-3.15	114.33	120.05
2	A	350	P4P	C4A-C5A-C6A	-3.11	115.64	120.19
2	A	350	P4P	C3A-C2A-C1A	-3.09	116.08	120.29
2	A	350	P4P	C3B-C2B-C1B	-2.96	116.27	120.29
2	C	750	P4P	C3B-C2B-C1B	-2.95	116.28	120.29
2	C	750	P4P	P-C1A-C6A	-2.67	115.19	120.05
2	A	350	P4P	P-C1A-C6A	-2.54	115.44	120.05
2	A	350	P4P	C1C-P-C1A	-2.52	104.59	109.44
2	C	750	P4P	C1C-P-C1A	-2.24	105.13	109.44
2	C	750	P4P	C1B-P-C1D	-2.23	105.15	109.44
2	C	750	P4P	C3D-C4D-C5D	2.24	123.86	119.93
2	A	350	P4P	P-C1B-C6B	2.25	124.13	120.05
2	A	350	P4P	C3D-C4D-C5D	2.26	123.89	119.93
2	C	750	P4P	P-C1B-C6B	2.26	124.15	120.05
2	A	350	P4P	C5A-C4A-C3A	2.45	124.24	119.93
2	C	750	P4P	C5A-C4A-C3A	2.49	124.30	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	750	P4P	P-C1C-C6C	3.67	126.70	120.05
2	A	350	P4P	P-C1C-C6C	3.69	126.74	120.05
2	C	750	P4P	C1D-P-C1C	3.74	116.62	109.44
2	A	350	P4P	C1D-P-C1C	3.74	116.62	109.44
2	A	350	P4P	C6A-C1A-C2A	3.92	124.38	118.91
2	C	750	P4P	C6A-C1A-C2A	4.09	124.61	118.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	P4P	1	0
2	C	750	P4P	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	95/110 (86%)	7.24	83 (87%) 0 1	74, 179, 296, 296	0
1	B	87/110 (79%)	7.12	70 (80%) 0 1	63, 171, 296, 296	0
1	C	95/110 (86%)	7.22	83 (87%) 0 1	68, 169, 296, 296	0
1	D	87/110 (79%)	7.26	71 (81%) 0 1	69, 166, 296, 296	0
All	All	364/440 (82%)	7.21	307 (84%) 0 1	63, 172, 296, 296	0

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	24	SER	27.5
1	B	24	SER	26.4
1	C	30	LEU	25.1
1	A	30	LEU	23.7
1	A	51	LEU	21.7
1	B	82	ARG	20.9
1	C	51	LEU	19.8
1	D	82	ARG	19.8
1	D	81	GLN	19.0
1	D	69	VAL	18.7
1	B	69	VAL	18.3
1	B	81	GLN	18.0
1	B	84	ASP	17.7
1	D	39	CYS	17.7
1	A	93	LEU	17.6
1	C	34	VAL	16.4
1	C	31	TRP	16.2
1	A	31	TRP	16.2
1	C	81	GLN	16.0
1	D	7	LEU	15.9
1	A	34	VAL	15.8

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Mol	Chain	Res	Type	RSRZ
1	C	89	ILE	15.0
1	A	81	GLN	14.8
1	A	90	GLY	14.8
1	B	39	CYS	14.7
1	C	93	LEU	14.7
1	D	54	ILE	14.7
1	B	28	THR	14.6
1	C	77	GLY	14.6
1	A	76	TRP	14.6
1	A	50	THR	14.4
1	A	23	PHE	14.4
1	A	94	ILE	14.3
1	C	23	PHE	14.1
1	C	50	THR	14.1
1	C	9	GLY	14.1
1	B	85	LEU	13.9
1	D	23	PHE	13.8
1	D	28	THR	13.7
1	B	80	GLY	13.6
1	B	23	PHE	13.5
1	C	76	TRP	13.4
1	C	100	ILE	13.4
1	D	38	ILE	13.2
1	D	52	ALA	12.9
1	D	85	LEU	12.9
1	A	91	MET	12.9
1	A	100	ILE	12.8
1	A	37	ILE	12.8
1	B	58	ILE	12.6
1	A	24	SER	12.5
1	B	52	ALA	12.4
1	D	80	GLY	12.3
1	B	55	PRO	12.3
1	D	58	ILE	12.2
1	A	9	GLY	12.2
1	A	75	SER	12.2
1	A	28	THR	12.2
1	D	32	PRO	12.1
1	B	32	PRO	12.1
1	D	77	GLY	12.0
1	A	85	LEU	12.0
1	A	89	ILE	12.0

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Mol	Chain	Res	Type	RSRZ
1	C	46	LEU	11.9
1	C	37	ILE	11.8
1	B	54	ILE	11.8
1	A	80	GLY	11.7
1	B	38	ILE	11.6
1	D	12	LEU	11.6
1	C	99	LEU	11.6
1	C	36	THR	11.5
1	B	12	LEU	11.5
1	C	86	PRO	11.4
1	B	73	LEU	11.4
1	A	32	PRO	11.4
1	B	70	LEU	11.3
1	C	24	SER	11.3
1	C	28	THR	11.3
1	A	86	PRO	11.2
1	D	73	LEU	11.1
1	D	70	LEU	11.0
1	A	46	LEU	11.0
1	D	8	GLY	10.9
1	B	31	TRP	10.8
1	A	83	LEU	10.8
1	B	76	TRP	10.7
1	C	85	LEU	10.7
1	B	33	SER	10.6
1	A	27	PHE	10.5
1	A	99	LEU	10.5
1	B	8	GLY	10.4
1	D	33	SER	10.4
1	C	32	PRO	10.3
1	D	19	THR	10.3
1	B	77	GLY	10.3
1	B	42	ALA	10.2
1	B	19	THR	10.1
1	C	80	GLY	10.1
1	D	42	ALA	10.1
1	C	101	ILE	10.0
1	D	84	ASP	9.9
1	D	50	THR	9.9
1	D	31	TRP	9.7
1	D	46	LEU	9.6
1	C	52	ALA	9.6

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Mol	Chain	Res	Type	RSRZ
1	B	50	THR	9.5
1	A	54	ILE	9.5
1	C	78	PHE	9.5
1	C	82	ARG	9.5
1	D	14	GLU	9.5
1	C	27	PHE	9.4
1	C	87	ALA	9.4
1	C	17	GLY	9.3
1	D	36	THR	9.3
1	C	7	LEU	9.3
1	A	52	ALA	9.2
1	D	76	TRP	9.1
1	A	36	THR	9.1
1	C	67	GLY	8.9
1	C	38	ILE	8.9
1	C	83	LEU	8.9
1	B	36	THR	8.9
1	D	29	ARG	8.8
1	B	51	LEU	8.8
1	B	93	LEU	8.8
1	C	84	ASP	8.8
1	B	29	ARG	8.6
1	B	87	ALA	8.5
1	D	21	MET	8.4
1	A	82	ARG	8.3
1	D	93	LEU	8.2
1	C	91	MET	8.2
1	A	95	CYS	8.2
1	B	21	MET	8.2
1	B	46	LEU	8.1
1	C	95	CYS	8.1
1	D	87	ALA	8.0
1	C	90	GLY	8.0
1	D	43	SER	8.0
1	B	30	LEU	7.9
1	A	84	ASP	7.8
1	C	54	ILE	7.8
1	A	20	LEU	7.7
1	D	30	LEU	7.6
1	B	56	THR	7.6
1	A	7	LEU	7.6
1	A	67	GLY	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	101	ILE	7.5
1	B	91	MET	7.4
1	D	16	ILE	7.4
1	D	79	PHE	7.3
1	D	56	THR	7.3
1	A	53	TYR	7.2
1	A	78	PHE	7.2
1	A	62	ILE	7.2
1	B	61	ALA	7.1
1	D	66	VAL	7.1
1	D	91	MET	7.1
1	A	25	GLU	7.0
1	A	74	LEU	7.0
1	C	20	LEU	7.0
1	A	29	ARG	6.9
1	D	61	ALA	6.9
1	D	57	GLY	6.9
1	C	94	ILE	6.9
1	C	55	PRO	6.9
1	A	55	PRO	6.9
1	C	62	ILE	6.9
1	B	66	VAL	6.8
1	C	53	TYR	6.8
1	C	74	LEU	6.8
1	B	43	SER	6.8
1	D	51	LEU	6.8
1	C	69	VAL	6.8
1	C	56	THR	6.8
1	B	15	VAL	6.7
1	A	58	ILE	6.7
1	C	25	GLU	6.6
1	C	8	GLY	6.6
1	B	14	GLU	6.5
1	A	49	GLN	6.5
1	D	64	SER	6.5
1	B	79	PHE	6.5
1	C	49	GLN	6.5
1	C	18	THR	6.5
1	C	96	ALA	6.5
1	B	57	GLY	6.4
1	A	38	ILE	6.4
1	C	58	ILE	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	7	LEU	6.3
1	C	75	SER	6.2
1	A	17	GLY	6.2
1	B	53	TYR	6.1
1	A	56	THR	6.1
1	C	29	ARG	6.0
1	A	96	ALA	6.0
1	A	18	THR	6.0
1	A	8	GLY	6.0
1	D	15	VAL	5.9
1	D	11	ILE	5.9
1	B	18	THR	5.9
1	A	61	ALA	5.9
1	D	55	PRO	5.8
1	B	16	ILE	5.8
1	A	35	GLY	5.8
1	D	13	ALA	5.8
1	C	71	ILE	5.7
1	D	89	ILE	5.7
1	A	69	VAL	5.6
1	A	65	GLY	5.5
1	B	11	ILE	5.4
1	D	18	THR	5.4
1	A	79	PHE	5.3
1	C	45	TRP	5.3
1	A	45	TRP	5.3
1	C	72	SER	5.3
1	B	13	ALA	5.3
1	A	87	ALA	5.2
1	D	53	TYR	5.2
1	D	78	PHE	5.2
1	A	77	GLY	5.2
1	C	65	GLY	5.2
1	B	64	SER	5.1
1	D	40	TYR	5.1
1	A	64	SER	5.1
1	C	79	PHE	4.8
1	A	71	ILE	4.8
1	C	41	CYS	4.8
1	A	41	CYS	4.7
1	C	13	ALA	4.7
1	B	83	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	35	GLY	4.6
1	B	78	PHE	4.6
1	D	65	GLY	4.6
1	B	40	TYR	4.6
1	C	14	GLU	4.6
1	A	13	ALA	4.5
1	A	14	GLU	4.5
1	D	45	TRP	4.5
1	B	67	GLY	4.4
1	B	71	ILE	4.4
1	B	65	GLY	4.4
1	B	75	SER	4.4
1	A	15	VAL	4.3
1	D	67	GLY	4.2
1	B	44	PHE	4.2
1	D	71	ILE	4.1
1	D	17	GLY	4.1
1	B	45	TRP	4.1
1	A	22	LYS	4.0
1	A	21	MET	4.0
1	C	22	LYS	4.0
1	A	73	LEU	3.9
1	D	27	PHE	3.9
1	D	83	LEU	3.9
1	C	15	VAL	3.9
1	B	17	GLY	3.8
1	B	27	PHE	3.8
1	C	39	CYS	3.6
1	A	39	CYS	3.6
1	D	88	ILE	3.6
1	D	37	ILE	3.5
1	D	44	PHE	3.5
1	B	22	LYS	3.5
1	D	49	GLN	3.5
1	C	88	ILE	3.4
1	D	22	LYS	3.4
1	C	92	MET	3.3
1	D	75	SER	3.3
1	C	64	SER	3.3
1	A	26	GLY	3.2
1	C	48	ALA	3.2
1	A	48	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	70	LEU	3.1
1	A	98	VAL	3.1
1	B	88	ILE	3.1
1	C	61	ALA	3.0
1	A	11	ILE	3.0
1	B	49	GLN	3.0
1	B	37	ILE	3.0
1	D	25	GLU	2.9
1	C	98	VAL	2.9
1	B	89	ILE	2.9
1	C	43	SER	2.8
1	A	43	SER	2.8
1	D	92	MET	2.8
1	A	63	TRP	2.7
1	B	92	MET	2.7
1	A	72	SER	2.7
1	A	70	LEU	2.7
1	B	68	ILE	2.6
1	C	63	TRP	2.6
1	B	90	GLY	2.6
1	C	10	ALA	2.6
1	A	68	ILE	2.5
1	C	21	MET	2.5
1	C	11	ILE	2.4
1	A	47	LEU	2.4
1	C	44	PHE	2.3
1	A	10	ALA	2.2
1	D	90	GLY	2.2
1	A	44	PHE	2.2
1	A	59	ALA	2.1
1	C	68	ILE	2.1
1	C	59	ALA	2.1
1	C	73	LEU	2.1
1	D	68	ILE	2.1

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 [i](#)

There are no carbohydrates 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. 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	P4P	A	350	25/25	0.71	0.63	-	140,140,140,140	0
2	P4P	C	750	25/25	0.71	0.62	-	133,133,133,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.