



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 10:09 PM UTC

PDB ID : 4LRV / pdb_00004lrv
Title : Crystal structure of DndE from Escherichia coli B7A involved in DNA phosphorothioation modification
Authors : Hu, W.; Wang, C.K.; Liang, J.D.; Zhang, T.L.; Yang, M.; Hu, Z.P.; Wang, Z.J.; Lan, W.X.; Wu, H.M.; Ding, J.P.; Wu, G.; Deng, Z.X.; Cao, C.
Deposited on : 2013-07-21
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

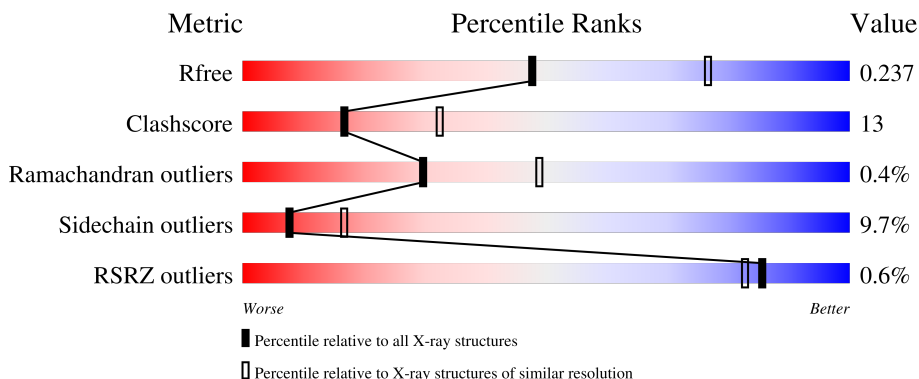
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	109	
1	B	109	
1	C	109	
1	D	109	
1	E	109	

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Mol	Chain	Length	Quality of chain
1	F	109	 66% 23% 6% 5%
1	G	109	 2% 68% 25% 6% 3%
1	H	109	 69% 22% 6% 3%
1	I	109	 59% 31% 6% 4%
1	J	109	 69% 24% 5% 2%
1	K	109	 71% 22% 5% 2%
1	L	109	 65% 25% 8% 2%
1	M	109	 64% 28% 6% 2%
1	N	109	 79% 14% 5% 2%
1	O	109	 71% 19% 7% 3%
1	P	109	 2% 64% 24% 7% 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13759 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 sulfur modification protein DndE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	107	Total 854	C 545	N 149	O 157	Se 3	0	0	0
1	B	106	Total 848	C 542	N 148	O 155	Se 3	0	0	0
1	C	105	Total 840	C 538	N 146	O 153	Se 3	0	0	0
1	D	107	Total 854	C 545	N 149	O 157	Se 3	0	0	0
1	E	102	Total 815	C 525	N 140	O 147	Se 3	0	0	0
1	F	104	Total 829	C 532	N 142	O 152	Se 3	0	0	0
1	G	106	Total 846	C 541	N 147	O 155	Se 3	0	0	0
1	H	106	Total 846	C 541	N 147	O 155	Se 3	0	0	0
1	I	102	Total 812	C 522	N 139	O 148	Se 3	0	0	0
1	J	106	Total 848	C 542	N 148	O 155	Se 3	0	0	0
1	K	104	Total 833	C 535	N 145	O 150	Se 3	0	0	0
1	L	100	Total 797	C 514	N 137	O 143	Se 3	0	0	0
1	M	106	Total 848	C 544	N 148	O 153	Se 3	0	0	0
1	N	104	Total 828	C 531	N 143	O 151	Se 3	0	0	0
1	O	106	Total 846	C 541	N 147	O 155	Se 3	0	0	0
1	P	104	Total 831	C 532	N 145	O 151	Se 3	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	expression tag	UNP B3HI59
B	2	SER	-	expression tag	UNP B3HI59
C	2	SER	-	expression tag	UNP B3HI59
D	2	SER	-	expression tag	UNP B3HI59
E	2	SER	-	expression tag	UNP B3HI59
F	2	SER	-	expression tag	UNP B3HI59
G	2	SER	-	expression tag	UNP B3HI59
H	2	SER	-	expression tag	UNP B3HI59
I	2	SER	-	expression tag	UNP B3HI59
J	2	SER	-	expression tag	UNP B3HI59
K	2	SER	-	expression tag	UNP B3HI59
L	2	SER	-	expression tag	UNP B3HI59
M	2	SER	-	expression tag	UNP B3HI59
N	2	SER	-	expression tag	UNP B3HI59
O	2	SER	-	expression tag	UNP B3HI59
P	2	SER	-	expression tag	UNP B3HI59

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	32	Total O 32 32	0	0
2	B	34	Total O 34 34	0	0
2	C	36	Total O 36 36	0	0
2	D	13	Total O 13 13	0	0
2	E	13	Total O 13 13	0	0
2	F	27	Total O 27 27	0	0
2	G	35	Total O 35 35	0	0
2	H	23	Total O 23 23	0	0
2	I	16	Total O 16 16	0	0
2	J	30	Total O 30 30	0	0
2	K	12	Total O 12 12	0	0

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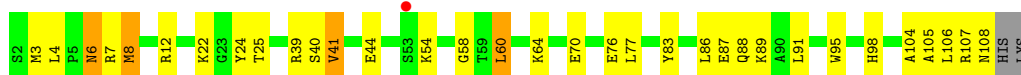
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	11	Total O 11 11	0	0
2	M	27	Total O 27 27	0	0
2	N	29	Total O 29 29	0	0
2	O	33	Total O 33 33	0	0
2	P	13	Total O 13 13	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

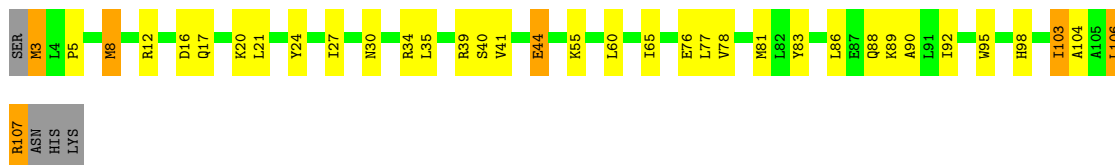
- Molecule 1: DNA sulfur modification protein DndE



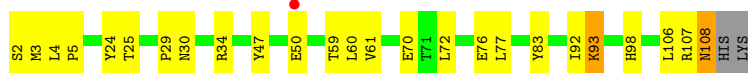
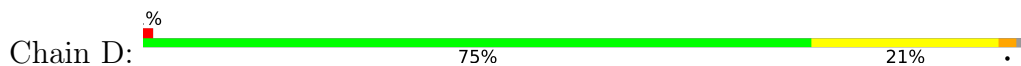
- Molecule 1: DNA sulfur modification protein DndE



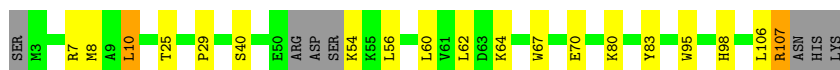
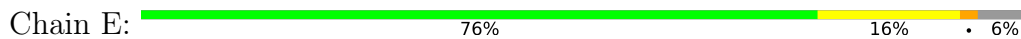
- Molecule 1: DNA sulfur modification protein DndE



- Molecule 1: DNA sulfur modification protein DndE

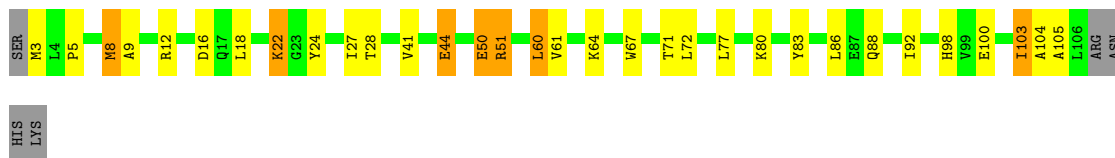


- Molecule 1: DNA sulfur modification protein DndE



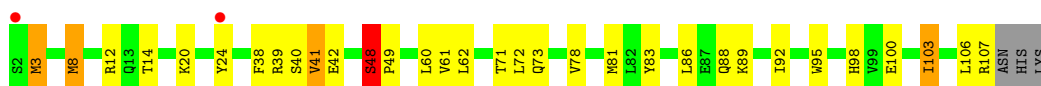
- Molecule 1: DNA sulfur modification protein DndE

Chain F: 



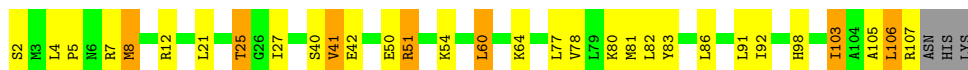
- Molecule 1: DNA sulfur modification protein DndE

Chain G: 



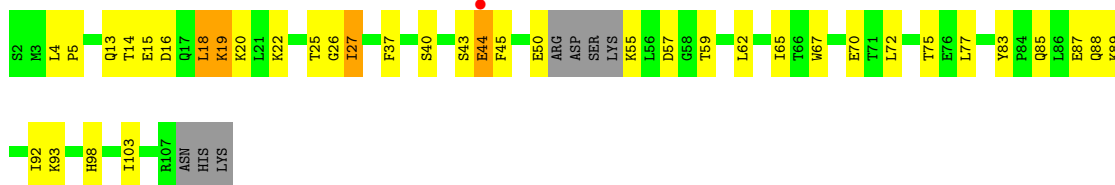
- Molecule 1: DNA sulfur modification protein DndE

Chain H: 



- Molecule 1: DNA sulfur modification protein DndE

Chain I: 



- Molecule 1: DNA sulfur modification protein DndE

Chain J: 

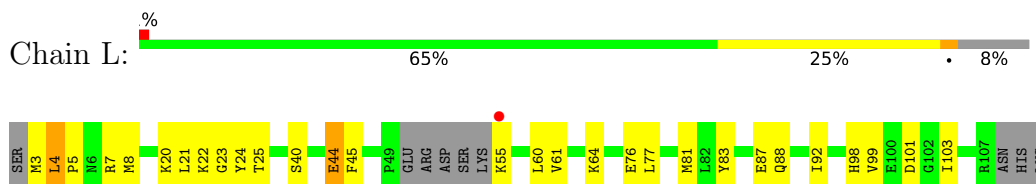


- Molecule 1: DNA sulfur modification protein DndE

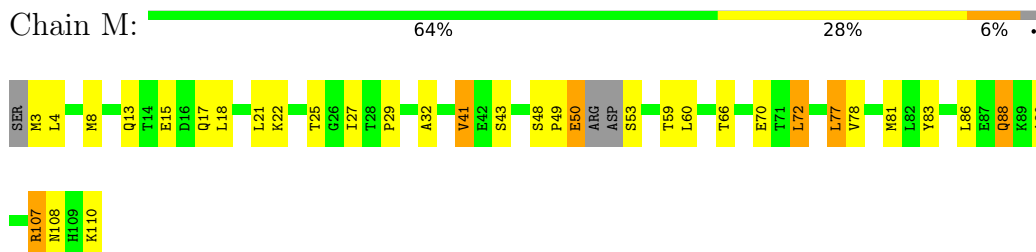
Chain K: 



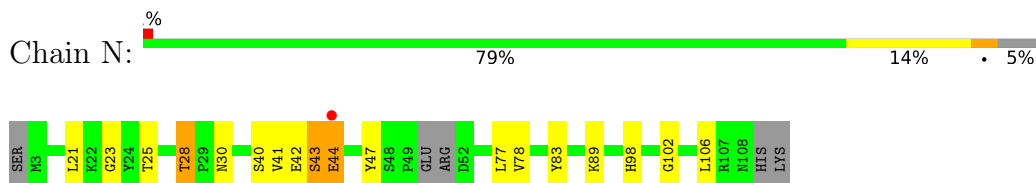
- Molecule 1: DNA sulfur modification protein DndE



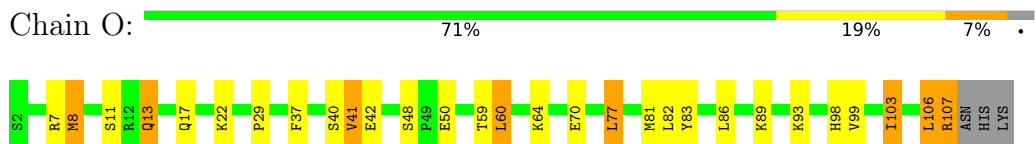
- Molecule 1: DNA sulfur modification protein DndE



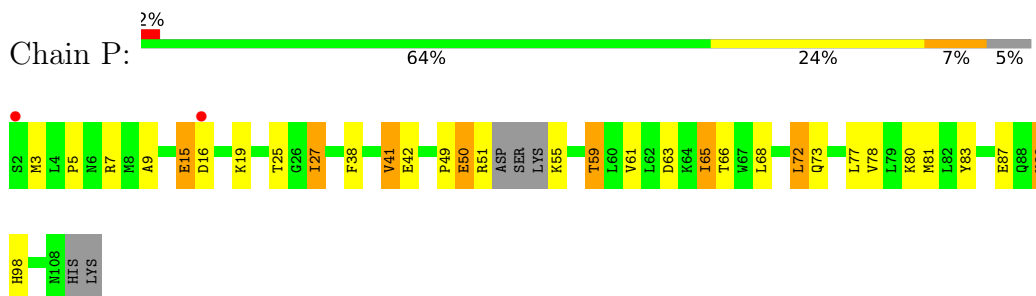
- Molecule 1: DNA sulfur modification protein DndE



- Molecule 1: DNA sulfur modification protein DndE



- Molecule 1: DNA sulfur modification protein DndE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.84Å 97.31Å 218.53Å 90.00° 95.81° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.3 (50.00-2.50) 88.3 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.54 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.201 , 0.242 0.198 , 0.237	Depositor DCC
R_{free} test set	3139 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtrriage
Anisotropy	0.147	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13759	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 30.81 % 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 1.2296e-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](#)

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	0.56	0/865	0.87	0/1161
1	B	0.51	0/860	0.83	1/1156 (0.1%)
1	C	0.52	0/852	0.84	0/1145
1	D	0.50	0/865	0.84	0/1161
1	E	0.52	0/826	0.89	0/1109
1	F	0.53	0/841	0.81	0/1131
1	G	0.52	0/857	0.91	2/1150 (0.2%)
1	H	0.51	0/857	0.82	0/1150
1	I	0.49	0/822	0.94	1/1103 (0.1%)
1	J	0.49	0/860	0.80	0/1156
1	K	0.52	0/845	0.90	0/1135
1	L	0.46	0/808	0.83	0/1086
1	M	0.51	0/860	0.81	0/1154
1	N	0.49	0/839	0.80	0/1127
1	O	0.49	0/857	0.84	3/1150 (0.3%)
1	P	0.49	0/841	0.85	0/1128
All	All	0.51	0/13555	0.85	7/18202 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	48	SER	CA-C-N	8.64	128.64	119.05
1	G	48	SER	C-N-CA	8.64	128.64	119.05
1	O	48	SER	CA-C-N	6.01	125.49	119.24
1	O	48	SER	C-N-CA	6.01	125.49	119.24
1	O	106	LEU	N-CA-C	-5.41	105.99	112.59

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	854	0	885	32	0
1	B	848	0	880	15	0
1	C	840	0	874	27	0
1	D	854	0	885	23	0
1	E	815	0	851	14	0
1	F	829	0	861	30	0
1	G	846	0	879	29	0
1	H	846	0	879	29	0
1	I	812	0	843	29	0
1	J	848	0	880	23	0
1	K	833	0	864	21	0
1	L	797	0	832	28	0
1	M	848	0	882	30	0
1	N	828	0	860	12	0
1	O	846	0	879	23	0
1	P	831	0	862	31	0
2	A	32	0	0	3	0
2	B	34	0	0	0	0
2	C	36	0	0	0	0
2	D	13	0	0	0	0
2	E	13	0	0	0	0
2	F	27	0	0	0	0
2	G	35	0	0	1	0
2	H	23	0	0	1	0
2	I	16	0	0	1	0
2	J	30	0	0	2	0
2	K	12	0	0	0	0
2	L	11	0	0	2	0
2	M	27	0	0	1	0
2	N	29	0	0	0	0
2	O	33	0	0	1	0
2	P	13	0	0	0	0
All	All	13759	0	13896	349	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 13.

The worst 5 of 349 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:I:5:PRO:CD	1:I:92:ILE:HD11	1.71	1.21
1:M:83:TYR:HB3	1:M:86:LEU:HD13	1.32	1.11
1:H:5:PRO:HD2	1:H:92:ILE:HD11	1.29	1.08
1:I:5:PRO:HD2	1:I:92:ILE:HD11	1.08	1.07
1:I:5:PRO:HD2	1:I:92:ILE:CD1	1.90	1.00

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	105/109 (96%)	100 (95%)	4 (4%)	1 (1%)	12	24
1	B	104/109 (95%)	99 (95%)	4 (4%)	1 (1%)	12	24
1	C	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
1	D	105/109 (96%)	98 (93%)	7 (7%)	0	100	100
1	E	98/109 (90%)	95 (97%)	3 (3%)	0	100	100
1	F	102/109 (94%)	97 (95%)	4 (4%)	1 (1%)	12	24
1	G	104/109 (95%)	100 (96%)	4 (4%)	0	100	100
1	H	104/109 (95%)	99 (95%)	4 (4%)	1 (1%)	12	24
1	I	98/109 (90%)	94 (96%)	3 (3%)	1 (1%)	12	24
1	J	104/109 (95%)	100 (96%)	4 (4%)	0	100	100
1	K	100/109 (92%)	96 (96%)	3 (3%)	1 (1%)	12	24
1	L	96/109 (88%)	91 (95%)	5 (5%)	0	100	100
1	M	102/109 (94%)	98 (96%)	4 (4%)	0	100	100
1	N	100/109 (92%)	98 (98%)	2 (2%)	0	100	100
1	O	104/109 (95%)	101 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	100/109 (92%)	94 (94%)	5 (5%)	1 (1%)	12	24
All	All	1629/1744 (93%)	1560 (96%)	62 (4%)	7 (0%)	30	49

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	88	GLN
1	A	105	ALA
1	B	105	ALA
1	F	104	ALA
1	H	106	LEU

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	91/90 (101%)	83 (91%)	8 (9%)	9	20
1	B	90/90 (100%)	79 (88%)	11 (12%)	5	10
1	C	89/90 (99%)	79 (89%)	10 (11%)	6	12
1	D	91/90 (101%)	82 (90%)	9 (10%)	7	16
1	E	86/90 (96%)	80 (93%)	6 (7%)	14	29
1	F	88/90 (98%)	78 (89%)	10 (11%)	5	12
1	G	90/90 (100%)	85 (94%)	5 (6%)	19	39
1	H	90/90 (100%)	79 (88%)	11 (12%)	5	10
1	I	86/90 (96%)	77 (90%)	9 (10%)	6	14
1	J	90/90 (100%)	79 (88%)	11 (12%)	5	10
1	K	88/90 (98%)	80 (91%)	8 (9%)	9	19
1	L	84/90 (93%)	78 (93%)	6 (7%)	13	29
1	M	90/90 (100%)	82 (91%)	8 (9%)	9	20
1	N	88/90 (98%)	82 (93%)	6 (7%)	14	31
1	O	90/90 (100%)	78 (87%)	12 (13%)	4	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	88/90 (98%)	80 (91%)	8 (9%)	9 19
All	All	1419/1440 (98%)	1281 (90%)	138 (10%)	8 17

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	43	SER
1	O	13	GLN
1	P	3	MSE
1	F	50	GLU
1	F	44	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	13	GLN
1	O	98	HIS
1	P	108	ASN
1	F	98	HIS
1	F	6	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [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	104/109 (95%)	-0.32	1 (0%) 79 76	11, 17, 29, 38	0
1	B	103/109 (94%)	-0.36	0 100 100	14, 19, 32, 44	0
1	C	102/109 (93%)	-0.30	0 100 100	12, 19, 30, 39	0
1	D	104/109 (95%)	-0.00	1 (0%) 79 76	16, 26, 45, 58	0
1	E	99/109 (90%)	-0.22	0 100 100	13, 22, 39, 49	0
1	F	101/109 (92%)	-0.25	0 100 100	16, 22, 33, 41	0
1	G	103/109 (94%)	-0.23	2 (1%) 66 62	15, 22, 34, 44	0
1	H	103/109 (94%)	-0.22	0 100 100	14, 22, 36, 47	0
1	I	99/109 (90%)	-0.04	1 (1%) 79 76	17, 26, 38, 50	0
1	J	103/109 (94%)	-0.24	0 100 100	16, 22, 34, 40	0
1	K	101/109 (92%)	-0.14	0 100 100	15, 22, 39, 46	0
1	L	97/109 (88%)	0.05	1 (1%) 79 76	18, 29, 43, 47	0
1	M	103/109 (94%)	-0.30	0 100 100	12, 20, 37, 45	0
1	N	101/109 (92%)	-0.34	1 (0%) 79 76	12, 21, 35, 40	0
1	O	103/109 (94%)	-0.30	0 100 100	14, 20, 35, 43	0
1	P	101/109 (92%)	-0.06	2 (1%) 65 61	16, 27, 44, 53	0
All	All	1627/1744 (93%)	-0.21	9 (0%) 85 83	11, 22, 38, 58	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	55	LYS	2.6
1	A	53	SER	2.3
1	P	16	ASP	2.2
1	D	50	GLU	2.1
1	G	2	SER	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.