



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:36 PM UTC

PDB ID : 4B7C / pdb_00004b7c
Title : Crystal structure of hypothetical protein PA1648 from *Pseudomonas aeruginosa*.
Authors : Alpey, M.S.; McMahon, S.A.; Duthie, F.G.; Naismith, J.H.
Deposited on : 2012-08-17
Resolution : 2.10 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)
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

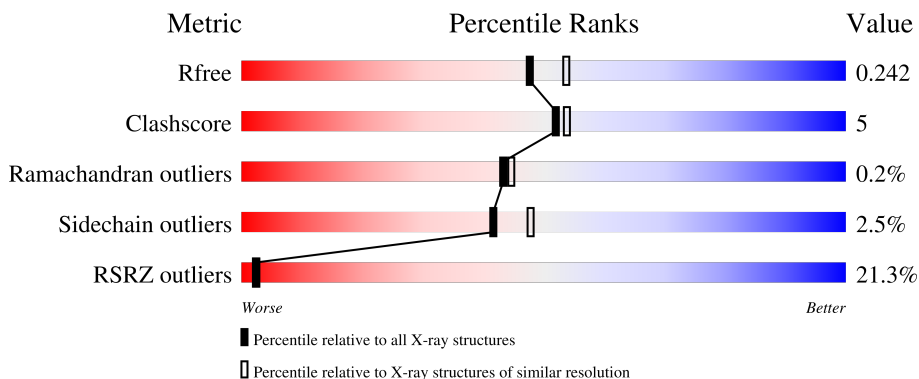
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	 10% 86% 10% ..
1	B	336	 19% 88% 10% ..
1	C	336	 20% 83% 12% ..
1	D	336	 4% 88% 9% .
1	E	336	 8% 87% 7% . 5%

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Mol	Chain	Length	Quality of chain
1	F	336	<p>22% 86% 10% ..</p>
1	G	336	<p>17% 85% 11% ..</p>
1	H	336	<p>20% 85% 10% 5%</p>
1	I	336	<p>22% 85% 9% ..</p>
1	J	336	<p>34% 78% 10% • 10%</p>
1	K	336	<p>54% 74% 10% • 15%</p>
1	L	336	<p>14% 83% 12% ..</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30125 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 PROBABLE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	325	Total 2473	C 1579	N 423	O 458	S 13	0	0	0
1	B	331	Total 2529	C 1613	N 437	O 466	S 13	0	1	0
1	C	323	Total 2450	C 1567	N 421	O 449	S 13	0	0	0
1	D	325	Total 2472	C 1579	N 423	O 457	S 13	0	0	0
1	E	320	Total 2424	C 1548	N 416	O 447	S 13	0	0	0
1	F	325	Total 2475	C 1581	N 425	O 456	S 13	0	0	0
1	G	323	Total 2452	C 1566	N 420	O 453	S 13	0	0	0
1	H	320	Total 2424	C 1548	N 415	O 448	S 13	0	0	0
1	I	323	Total 2454	C 1567	N 422	O 452	S 13	0	0	0
1	J	302	Total 2289	C 1463	N 392	O 422	S 12	0	0	0
1	K	286	Total 2172	C 1394	N 367	O 399	S 12	0	0	0
1	L	325	Total 2475	C 1581	N 425	O 456	S 13	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

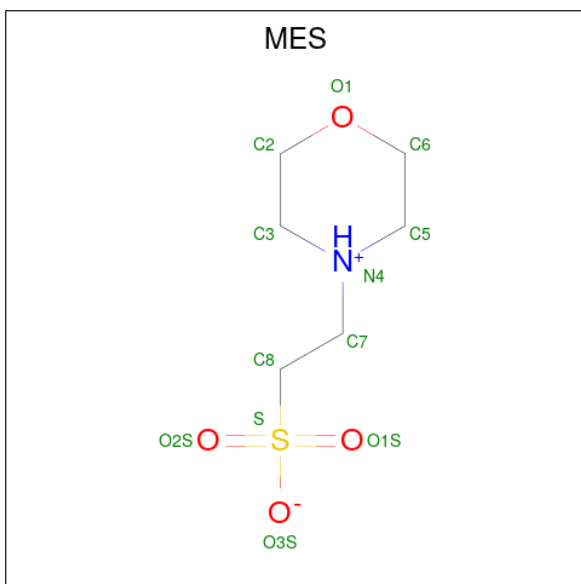
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B7UV73
A	0	ALA	-	expression tag	UNP B7UV73
B	-1	GLY	-	expression tag	UNP B7UV73
B	0	ALA	-	expression tag	UNP B7UV73
C	-1	GLY	-	expression tag	UNP B7UV73

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP B7UV73
D	-1	GLY	-	expression tag	UNP B7UV73
D	0	ALA	-	expression tag	UNP B7UV73
E	-1	GLY	-	expression tag	UNP B7UV73
E	0	ALA	-	expression tag	UNP B7UV73
F	-1	GLY	-	expression tag	UNP B7UV73
F	0	ALA	-	expression tag	UNP B7UV73
G	-1	GLY	-	expression tag	UNP B7UV73
G	0	ALA	-	expression tag	UNP B7UV73
H	-1	GLY	-	expression tag	UNP B7UV73
H	0	ALA	-	expression tag	UNP B7UV73
I	-1	GLY	-	expression tag	UNP B7UV73
I	0	ALA	-	expression tag	UNP B7UV73
J	-1	GLY	-	expression tag	UNP B7UV73
J	0	ALA	-	expression tag	UNP B7UV73
K	-1	GLY	-	expression tag	UNP B7UV73
K	0	ALA	-	expression tag	UNP B7UV73
L	-1	GLY	-	expression tag	UNP B7UV73
L	0	ALA	-	expression tag	UNP B7UV73

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			S
2	D	1	12	6	1	4	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

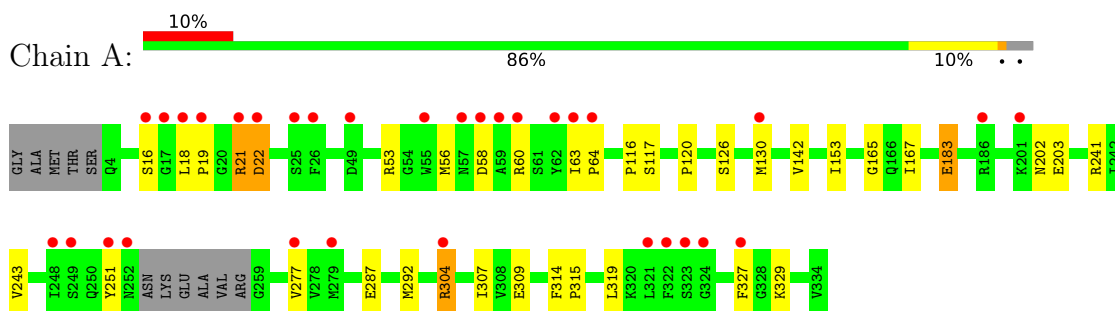
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	88	Total	O	0	0
			88	88		
3	C	77	Total	O	0	0
			77	77		
3	D	141	Total	O	0	0
			141	141		
3	E	132	Total	O	0	0
			132	132		
3	F	55	Total	O	0	0
			55	55		
3	G	87	Total	O	0	0
			87	87		
3	H	36	Total	O	0	0
			36	36		
3	I	48	Total	O	0	0
			48	48		
3	J	72	Total	O	0	0
			72	72		
3	K	24	Total	O	0	0
			24	24		
3	L	70	Total	O	0	0
			70	70		

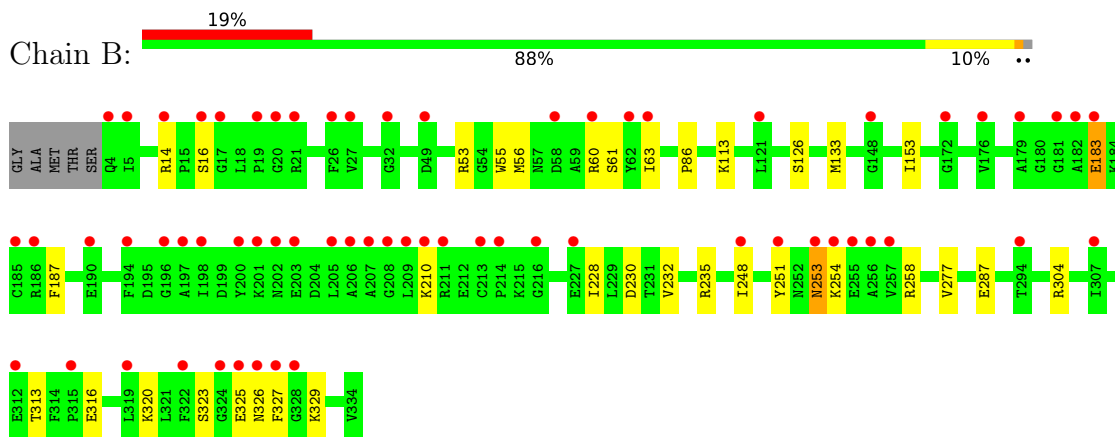
3 Residue-property plots [i](#)

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.

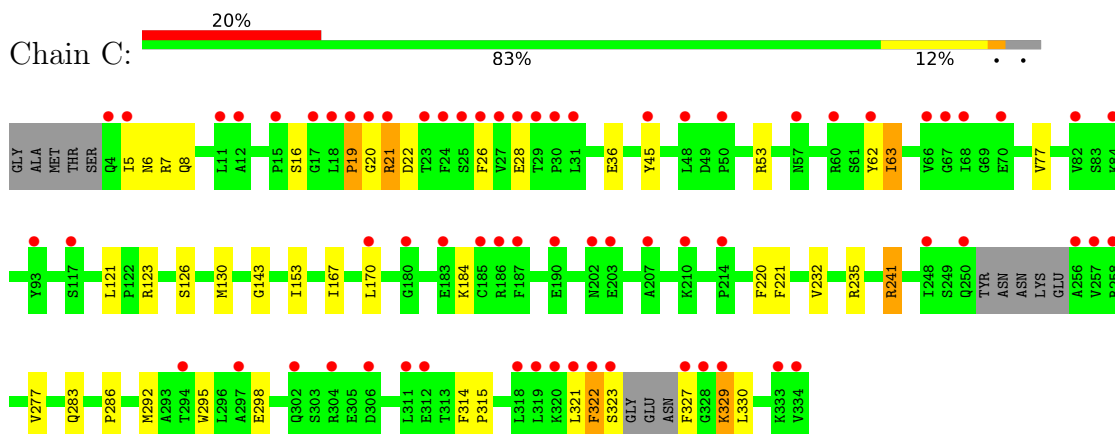
• Molecule 1: PROBABLE OXIDOREDUCTASE



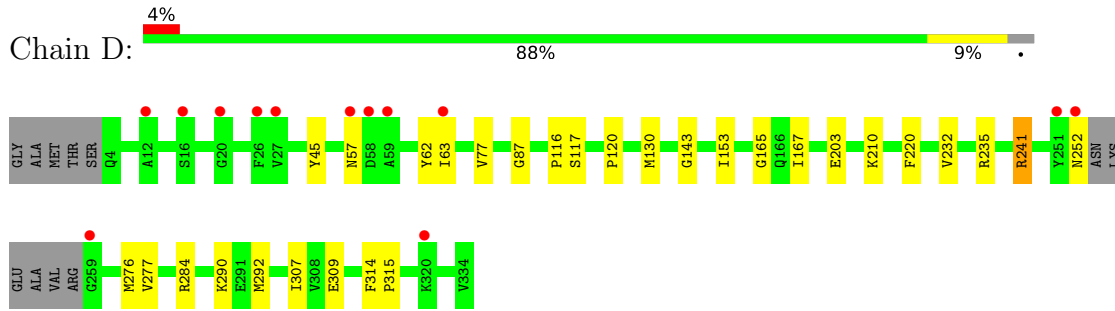
• Molecule 1: PROBABLE OXIDOREDUCTASE



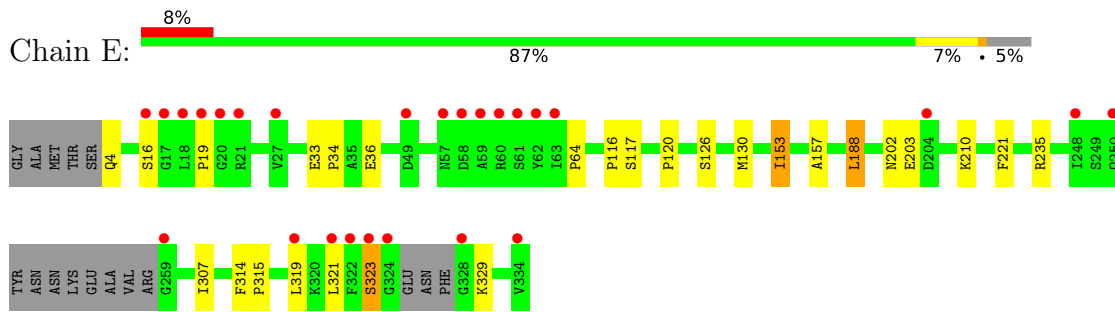
• Molecule 1: PROBABLE OXIDOREDUCTASE



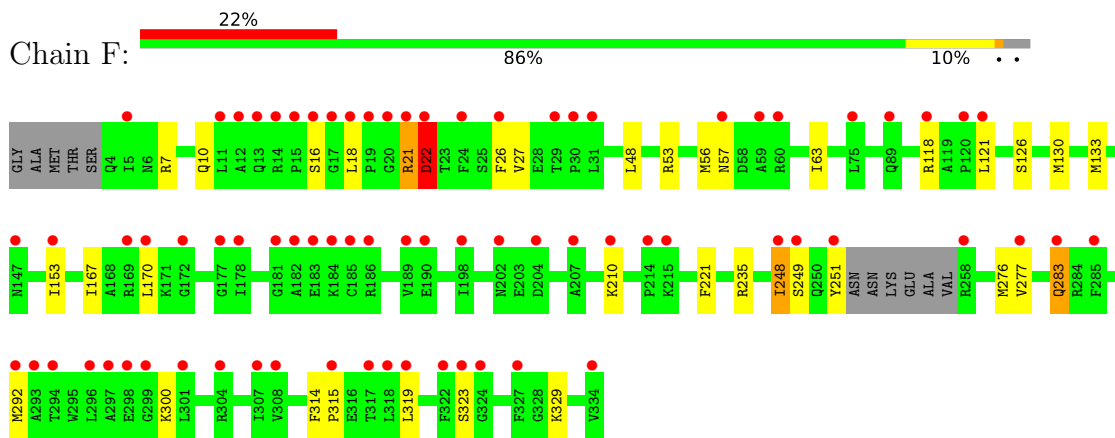
● Molecule 1: PROBABLE OXIDOREDUCTASE



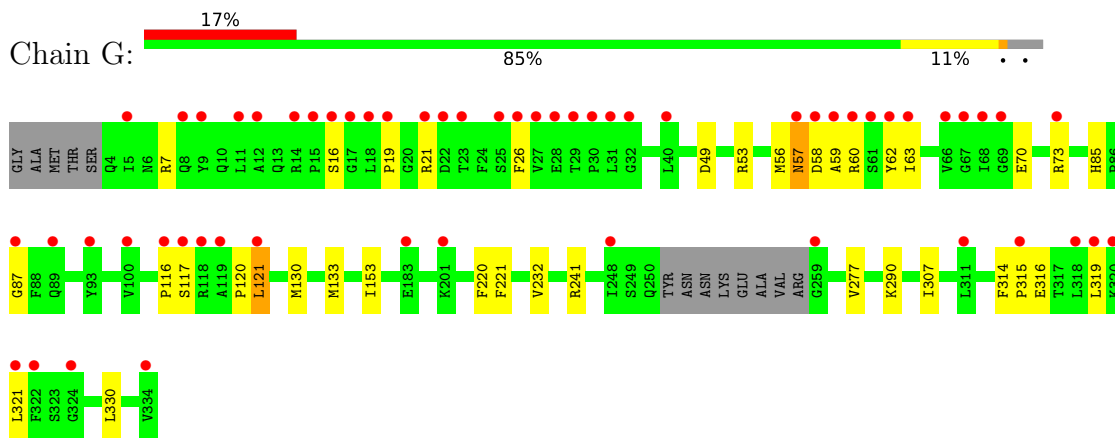
● Molecule 1: PROBABLE OXIDOREDUCTASE

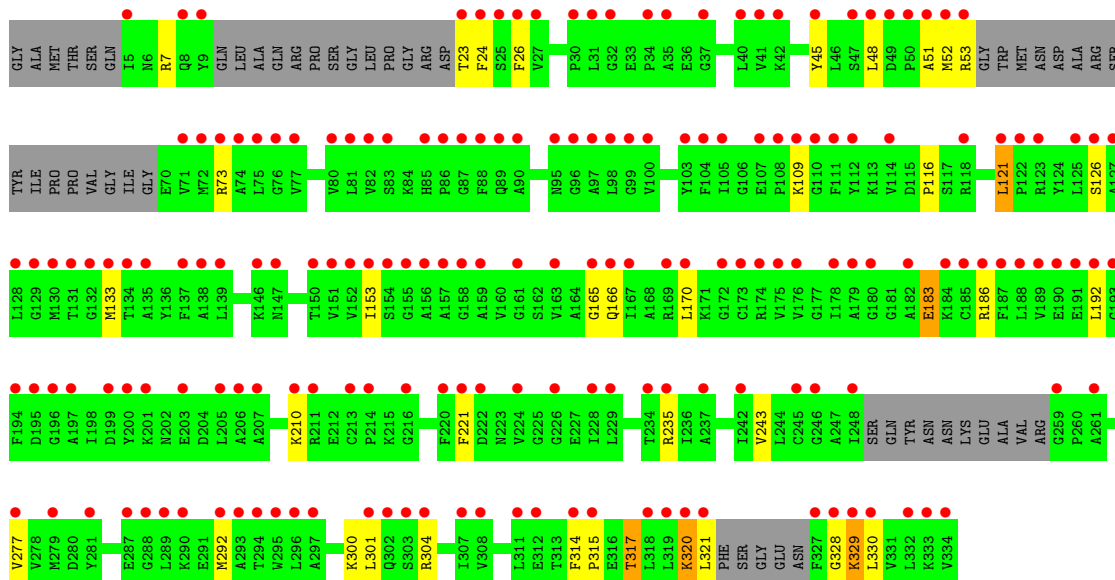


● Molecule 1: PROBABLE OXIDOREDUCTASE

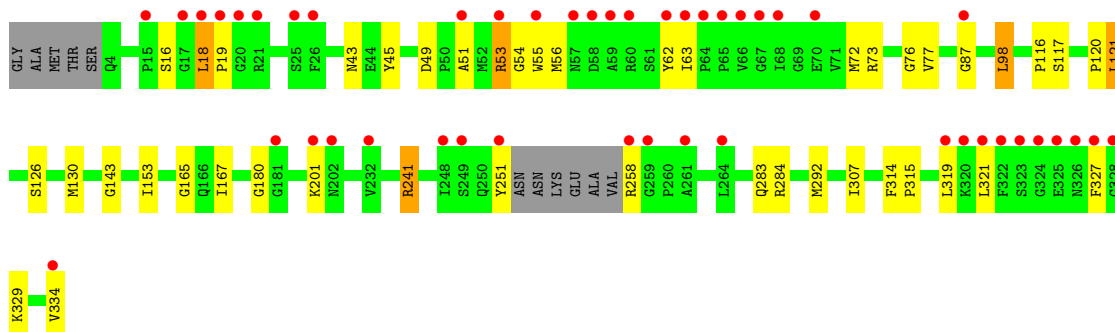
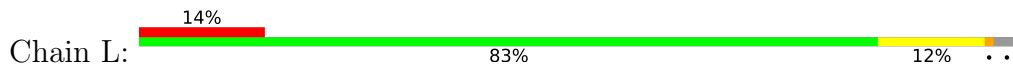


● Molecule 1: PROBABLE OXIDOREDUCTASE





● Molecule 1: PROBABLE OXIDOREDUCTASE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	170.93Å 177.09Å 181.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.06 – 2.10 73.06 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (73.06-2.10) 99.1 (73.06-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.223 , 0.243 0.224 , 0.242	Depositor DCC
R_{free} test set	16092 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtrriage
Anisotropy	0.180	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.015 for -h,l,k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30125	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MES

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	0.71	1/2520 (0.0%)	0.91	8/3401 (0.2%)
1	B	0.64	0/2580	0.82	1/3483 (0.0%)
1	C	0.68	0/2495	0.87	4/3367 (0.1%)
1	D	0.67	0/2519	0.85	7/3401 (0.2%)
1	E	0.68	1/2468 (0.0%)	0.81	0/3330
1	F	0.64	1/2522 (0.0%)	0.78	1/3404 (0.0%)
1	G	0.62	0/2498	0.79	2/3372 (0.1%)
1	H	0.62	0/2468	0.84	3/3330 (0.1%)
1	I	0.64	0/2500	0.84	4/3374 (0.1%)
1	J	0.64	0/2325	0.82	3/3128 (0.1%)
1	K	0.65	2/2207 (0.1%)	0.86	4/2972 (0.1%)
1	L	0.63	0/2522	0.86	5/3404 (0.1%)
All	All	0.65	5/29624 (0.0%)	0.84	42/39966 (0.1%)

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	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	64	PRO	CA-C	6.06	1.55	1.51
1	K	328	GLY	N-CA	5.97	1.54	1.45
1	F	22	ASP	CA-CB	5.52	1.61	1.53
1	K	186	ARG	CA-CB	5.35	1.61	1.53
1	A	64	PRO	CA-C	5.34	1.54	1.51

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ARG	NE-CZ-NH2	-11.36	108.97	119.20
1	C	241	ARG	NE-CZ-NH1	10.76	132.26	121.50
1	J	31	LEU	N-CA-C	10.26	125.67	112.34
1	L	284	ARG	NE-CZ-NH2	8.42	126.78	119.20
1	D	284	ARG	NE-CZ-NH2	8.37	126.73	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	19	PRO	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	2473	0	2491	21	1
1	B	2529	0	2557	24	0
1	C	2450	0	2481	29	1
1	D	2472	0	2491	24	0
1	E	2424	0	2454	18	1
1	F	2475	0	2498	25	0
1	G	2452	0	2476	29	0
1	H	2424	0	2452	24	0
1	I	2454	0	2481	25	0
1	J	2289	0	2322	41	0
1	K	2172	0	2210	31	1
1	L	2475	0	2498	38	0
2	D	12	0	13	0	0
2	F	12	0	13	0	0
2	G	12	0	13	0	0
2	H	12	0	13	2	0
2	I	12	0	13	2	0
3	A	146	0	0	0	0
3	B	88	0	0	1	0
3	C	77	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	141	0	0	1	0
3	E	132	0	0	2	0
3	F	55	0	0	2	0
3	G	87	0	0	2	0
3	H	36	0	0	0	0
3	I	48	0	0	0	0
3	J	72	0	0	0	0
3	K	24	0	0	0	0
3	L	70	0	0	0	0
All	All	30125	0	29476	297	2

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.

The worst 5 of 297 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:B:323:SER:OG	1:B:325:GLU:HB2	1.58	1.01
1:J:52:MET:C	1:J:54:GLY:H	1.76	0.89
1:E:130:MET:HE3	3:E:2040:HOH:O	1.80	0.82
1:K:321:LEU:HD13	1:K:330:LEU:HD23	1.62	0.82
1:C:36:GLU:CG	1:J:5:ILE:HD12	2.16	0.76

All (2) 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:202:ASN:OD1	1:K:45:TYR:OH[2_554]	1.54	0.66
1:C:45:TYR:OH	1:E:202:ASN:OD1[3_655]	1.58	0.62

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	321/336 (96%)	317 (99%)	4 (1%)	0	100	100
1	B	330/336 (98%)	324 (98%)	6 (2%)	0	100	100
1	C	317/336 (94%)	311 (98%)	4 (1%)	2 (1%)	21	18
1	D	321/336 (96%)	317 (99%)	4 (1%)	0	100	100
1	E	314/336 (94%)	309 (98%)	4 (1%)	1 (0%)	36	36
1	F	321/336 (96%)	317 (99%)	4 (1%)	0	100	100
1	G	319/336 (95%)	315 (99%)	4 (1%)	0	100	100
1	H	314/336 (94%)	307 (98%)	7 (2%)	0	100	100
1	I	319/336 (95%)	309 (97%)	9 (3%)	1 (0%)	36	36
1	J	292/336 (87%)	286 (98%)	5 (2%)	1 (0%)	36	36
1	K	276/336 (82%)	269 (98%)	6 (2%)	1 (0%)	30	28
1	L	321/336 (96%)	316 (98%)	5 (2%)	0	100	100
All	All	3765/4032 (93%)	3697 (98%)	62 (2%)	6 (0%)	43	44

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	53	ARG
1	C	21	ARG
1	C	322	PHE
1	E	323	SER
1	I	327	PHE

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	255/263 (97%)	245 (96%)	10 (4%)	28	31
1	B	261/263 (99%)	256 (98%)	5 (2%)	50	58
1	C	252/263 (96%)	246 (98%)	6 (2%)	43	49
1	D	255/263 (97%)	253 (99%)	2 (1%)	73	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	250/263 (95%)	243 (97%)	7 (3%)	38	43
1	F	255/263 (97%)	246 (96%)	9 (4%)	32	35
1	G	253/263 (96%)	247 (98%)	6 (2%)	43	49
1	H	250/263 (95%)	250 (100%)	0	100	100
1	I	253/263 (96%)	246 (97%)	7 (3%)	38	43
1	J	235/263 (89%)	225 (96%)	10 (4%)	26	27
1	K	224/263 (85%)	218 (97%)	6 (3%)	39	45
1	L	255/263 (97%)	247 (97%)	8 (3%)	35	39
All	All	2998/3156 (95%)	2922 (98%)	76 (2%)	42	48

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	121	LEU
1	L	98	LEU
1	J	250	GLN
1	K	277	VAL
1	L	327	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	302	GLN
1	K	223	ASN
1	L	223	ASN
1	E	283	GLN
1	D	302	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 [i](#)

5 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	MES	G	1335	-	12,12,12	2.13	1 (8%)	15,16,16	1.73	3 (20%)
2	MES	H	1335	-	12,12,12	2.15	1 (8%)	15,16,16	5.82	7 (46%)
2	MES	I	1335	-	12,12,12	2.08	1 (8%)	15,16,16	5.73	6 (40%)
2	MES	D	1335	-	12,12,12	1.64	1 (8%)	15,16,16	1.73	4 (26%)
2	MES	F	1335	-	12,12,12	2.01	1 (8%)	15,16,16	5.59	9 (60%)

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	MES	G	1335	-	-	1/6/14/14	0/1/1/1
2	MES	H	1335	-	-	3/6/14/14	0/1/1/1
2	MES	I	1335	-	-	2/6/14/14	0/1/1/1
2	MES	D	1335	-	-	1/6/14/14	0/1/1/1
2	MES	F	1335	-	-	2/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1335	MES	C8-S	-6.88	1.67	1.77
2	G	1335	MES	C8-S	-6.81	1.68	1.77
2	I	1335	MES	C8-S	-6.68	1.68	1.77
2	F	1335	MES	C8-S	-6.20	1.68	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1335	MES	C8-S	-4.96	1.70	1.77

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1335	MES	O1S-S-C8	-12.70	87.54	106.73
2	I	1335	MES	O1S-S-C8	-12.63	87.65	106.73
2	H	1335	MES	O3S-S-O1S	-12.30	80.62	111.40
2	F	1335	MES	O1S-S-C8	-11.09	89.98	106.73
2	I	1335	MES	O3S-S-O1S	-10.98	83.93	111.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1335	MES	C8-C7-N4-C5
2	G	1335	MES	C8-C7-N4-C5
2	H	1335	MES	C7-C8-S-O3S
2	I	1335	MES	C7-C8-S-O2S
2	F	1335	MES	C7-C8-S-O3S

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1335	MES	2	0
2	I	1335	MES	2	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 [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	325/336 (96%)	0.40	32 (9%) 13 13	20, 31, 66, 88	0
1	B	331/336 (98%)	1.10	64 (19%) 3 3	19, 42, 70, 102	1 (0%)
1	C	323/336 (96%)	1.21	68 (21%) 2 2	26, 46, 77, 98	0
1	D	325/336 (96%)	0.26	13 (4%) 42 44	21, 32, 53, 73	0
1	E	320/336 (95%)	0.28	26 (8%) 18 19	20, 30, 61, 93	0
1	F	325/336 (96%)	1.32	75 (23%) 2 2	30, 49, 80, 101	0
1	G	323/336 (96%)	0.82	57 (17%) 4 4	23, 42, 77, 100	0
1	H	320/336 (95%)	1.34	68 (21%) 2 2	31, 54, 82, 102	0
1	I	323/336 (96%)	1.41	73 (22%) 2 2	33, 53, 83, 117	0
1	J	302/336 (89%)	1.54	114 (37%) 1 1	27, 45, 83, 109	0
1	K	286/336 (85%)	2.55	180 (62%) 0 0	39, 66, 99, 115	0
1	L	325/336 (96%)	0.85	46 (14%) 6 6	25, 39, 80, 118	0
All	All	3828/4032 (94%)	1.07	816 (21%) 2 2	19, 44, 81, 118	1 (0%)

The worst 5 of 816 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	68	ILE	8.6
1	B	327	PHE	8.2
1	J	324	GLY	7.7
1	J	24	PHE	7.5
1	K	327	PHE	7.4

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(\AA^2)	Q<0.9
2	MES	I	1335	12/12	0.86	0.17	61,65,73,73	0
2	MES	H	1335	12/12	0.88	0.17	73,75,77,78	0
2	MES	F	1335	12/12	0.92	0.15	41,51,52,53	0
2	MES	G	1335	12/12	0.94	0.11	40,41,41,42	0
2	MES	D	1335	12/12	0.97	0.08	28,32,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.