



wwPDB X-ray Structure Validation Summary Report

May 28, 2020 – 10:26 pm BST

PDB ID : 2JES
Title : Portal protein (gp6) from bacteriophage SPP1
Authors : Lebedev, A.A.; Krause, M.H.; Isidro, A.L.; Vagin, A.A.; Orlova, E.V.; Turner, J.; Dodson, E.J.; Tavares, P.; Antson, A.A.
Deposited on : 2007-01-21
Resolution : 3.40 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 following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

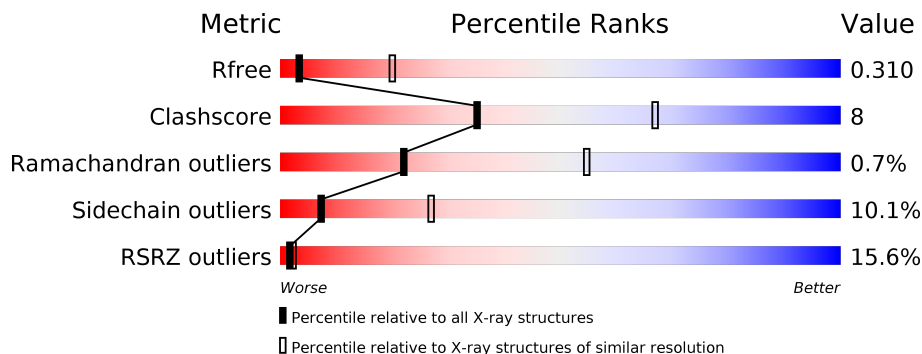
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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	503	 12% 58% 14% • 26%
1	C	503	 14% 56% 15% • 26%
1	E	503	 15% 58% 13% • 26%
1	G	503	 13% 55% 16% • 26%
1	I	503	 13% 55% 16% • 26%
1	K	503	 11% 54% 17% • 26%

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Mol	Chain	Length	Quality of chain
1	M	503	
1	O	503	
1	Q	503	
1	S	503	
1	U	503	
1	W	503	
1	Y	503	
2	B	30	
2	D	30	
2	F	30	
2	H	30	
2	J	30	
2	L	30	
2	N	30	
2	P	30	
2	R	30	
2	T	30	
2	V	30	
2	X	30	
2	Z	30	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 39260 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 PORTAL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	2868	1823	472	563	10	0	0	0
1	C	370	2868	1823	472	563	10	0	0	0
1	E	370	2868	1823	472	563	10	0	0	0
1	G	370	2868	1823	472	563	10	0	0	0
1	I	370	2868	1823	472	563	10	0	0	0
1	K	370	2868	1823	472	563	10	0	0	0
1	M	370	2868	1823	472	563	10	0	0	0
1	O	370	2868	1823	472	563	10	0	0	0
1	Q	370	2868	1823	472	563	10	0	0	0
1	S	370	2868	1823	472	563	10	0	0	0
1	U	370	2868	1823	472	563	10	0	0	0
1	W	370	2868	1823	472	563	10	0	0	0
1	Y	370	2868	1823	472	563	10	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	LYS	ASN	engineered mutation	UNP P54309
C	365	LYS	ASN	engineered mutation	UNP P54309
E	365	LYS	ASN	engineered mutation	UNP P54309

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Chain	Residue	Modelled	Actual	Comment	Reference
G	365	LYS	ASN	engineered mutation	UNP P54309
I	365	LYS	ASN	engineered mutation	UNP P54309
K	365	LYS	ASN	engineered mutation	UNP P54309
M	365	LYS	ASN	engineered mutation	UNP P54309
O	365	LYS	ASN	engineered mutation	UNP P54309
Q	365	LYS	ASN	engineered mutation	UNP P54309
S	365	LYS	ASN	engineered mutation	UNP P54309
U	365	LYS	ASN	engineered mutation	UNP P54309
W	365	LYS	ASN	engineered mutation	UNP P54309
Y	365	LYS	ASN	engineered mutation	UNP P54309

- Molecule 2 is a protein called UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	D	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	F	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	H	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	J	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	L	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	N	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	P	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	R	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	T	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	V	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	X	30	Total	C	N	O	0	0	0
			150	90	30	30			
2	Z	30	Total	C	N	O	0	0	0
			150	90	30	30			

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Hg 1 1	0	0
3	Q	1	Total Hg 1 1	0	0
3	K	1	Total Hg 1 1	0	0
3	E	1	Total Hg 1 1	0	0
3	I	1	Total Hg 1 1	0	0
3	C	1	Total Hg 1 1	0	0
3	W	1	Total Hg 1 1	0	0
3	A	1	Total Hg 1 1	0	0
3	U	1	Total Hg 1 1	0	0
3	O	1	Total Hg 1 1	0	0
3	Y	1	Total Hg 1 1	0	0
3	S	1	Total Hg 1 1	0	0
3	M	1	Total Hg 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Ca 1 1	0	0
4	Q	1	Total Ca 1 1	0	0
4	K	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	I	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	W	1	Total Ca 1 1	0	0

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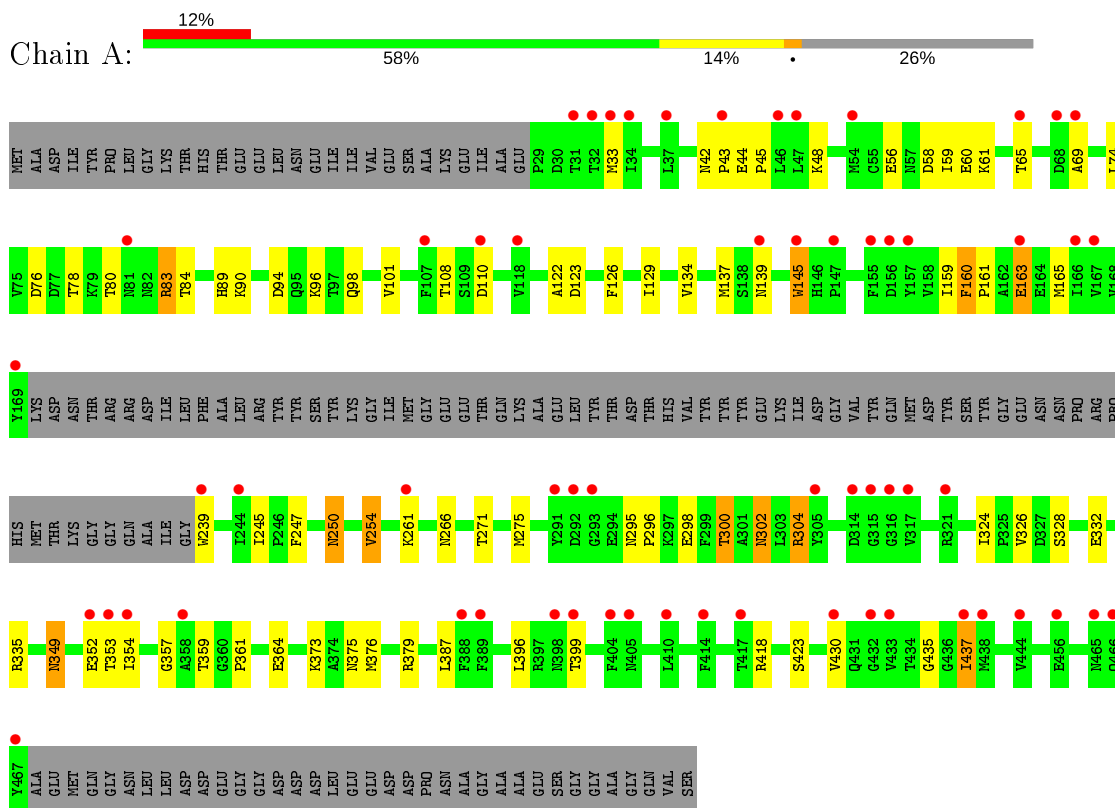
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	U	1	Total 1	Ca 1	0	0
4	O	1	Total 1	Ca 1	0	0
4	Y	1	Total 1	Ca 1	0	0
4	S	1	Total 1	Ca 1	0	0
4	M	1	Total 1	Ca 1	0	0

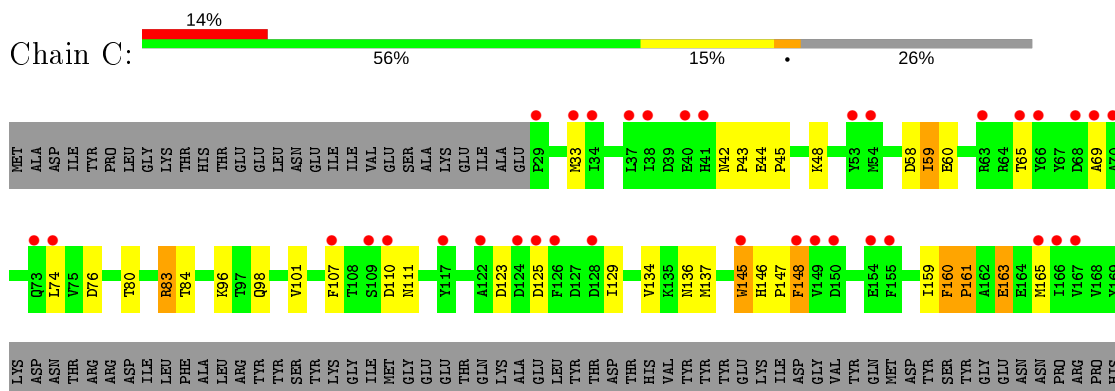
3 Residue-property plots [i](#)

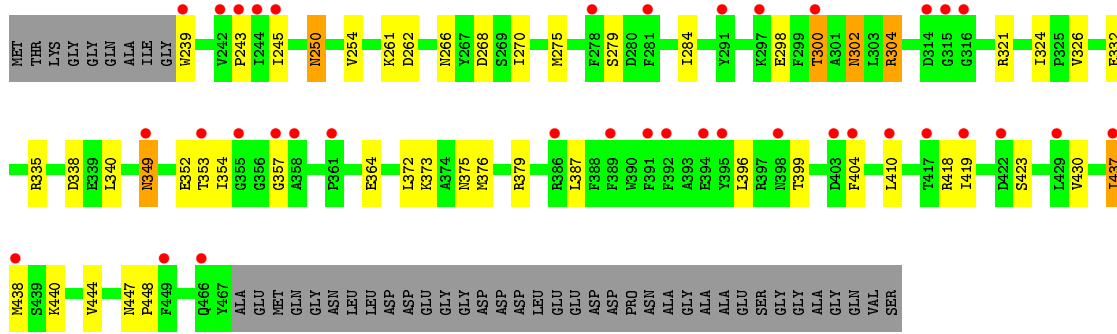
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: PORTAL PROTEIN

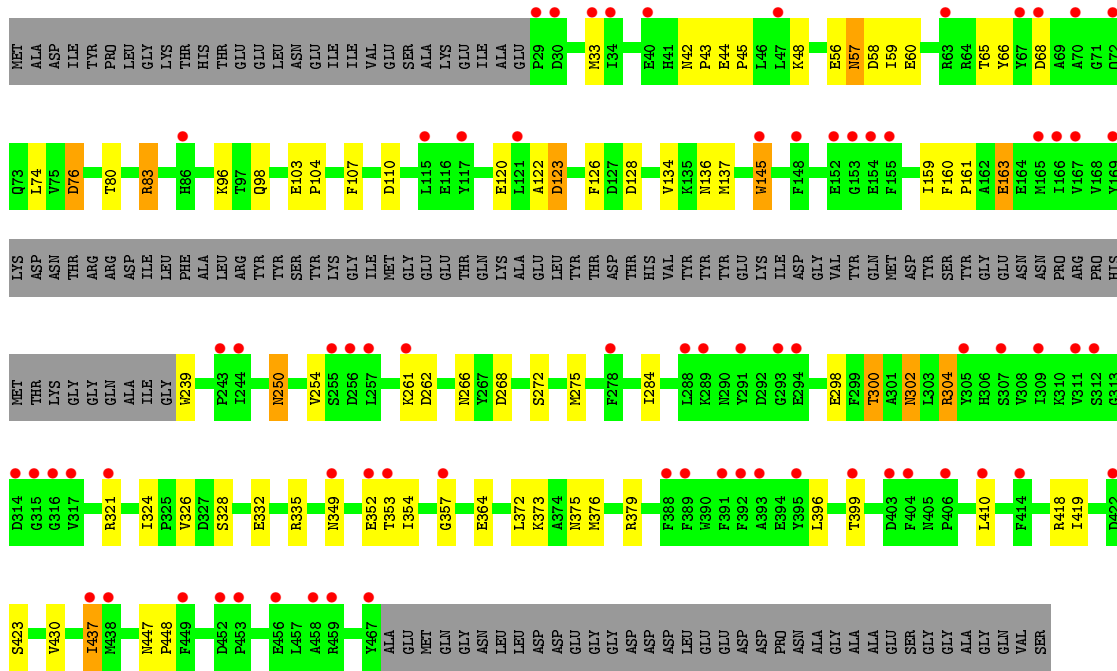


- Molecule 1: PORTAL PROTEIN

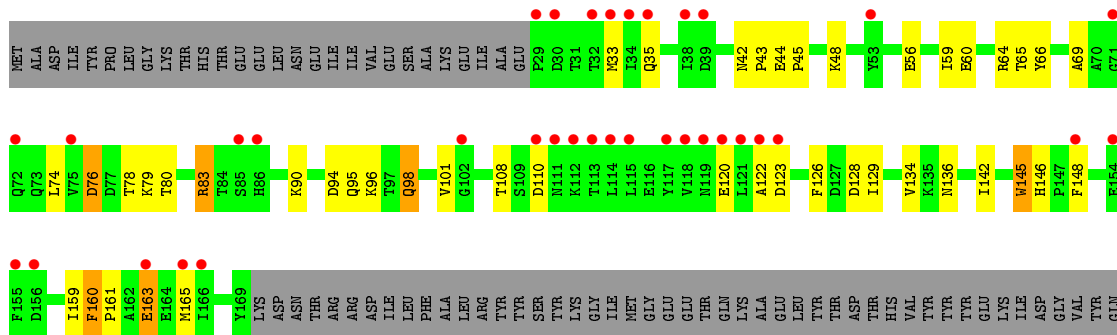


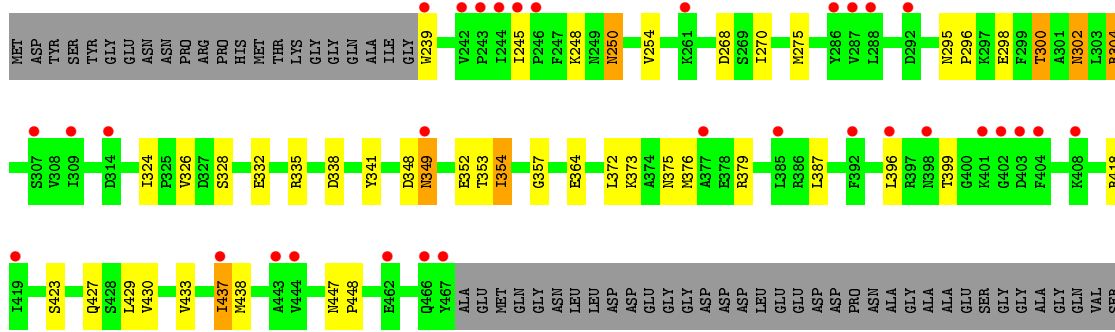


• Molecule 1: PORTAL PROTEIN

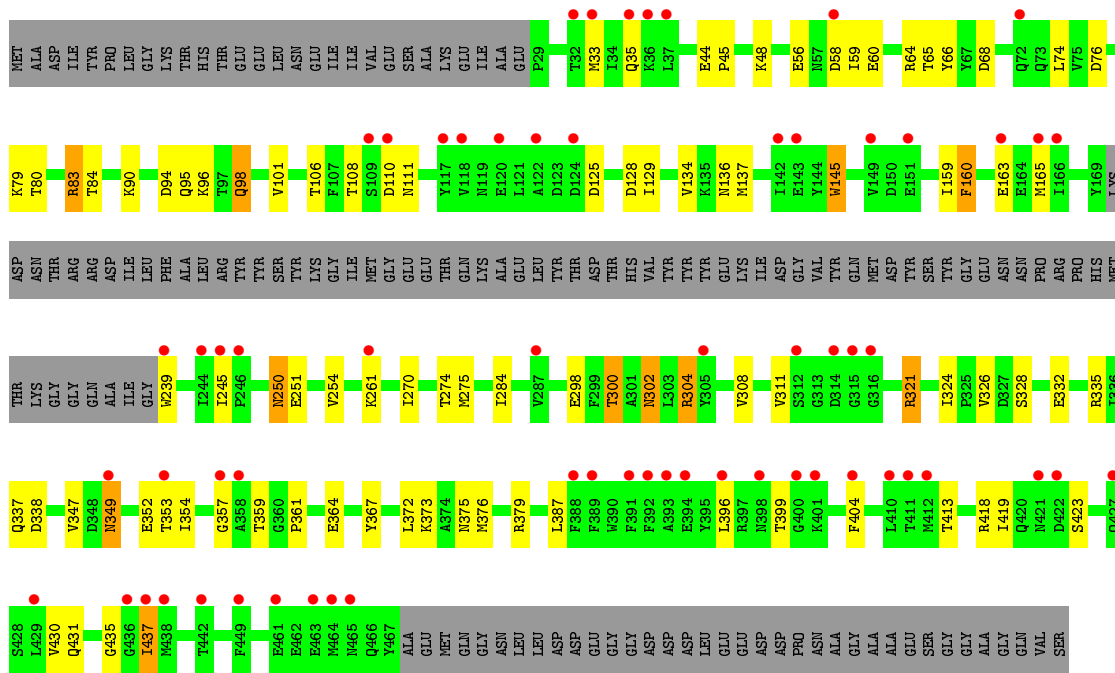


• Molecule 1: PORTAL PROTEIN

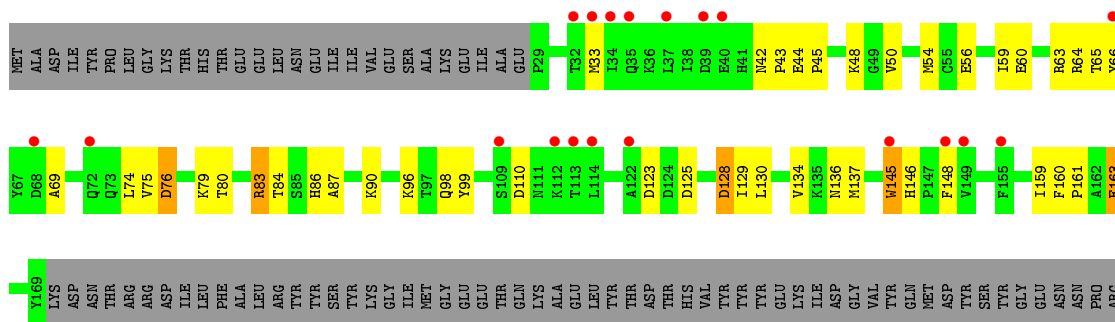


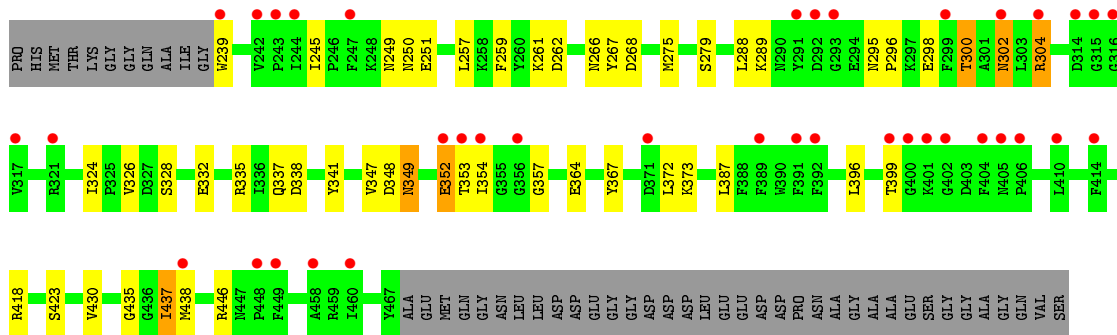


• Molecule 1: PORTAL PROTEIN

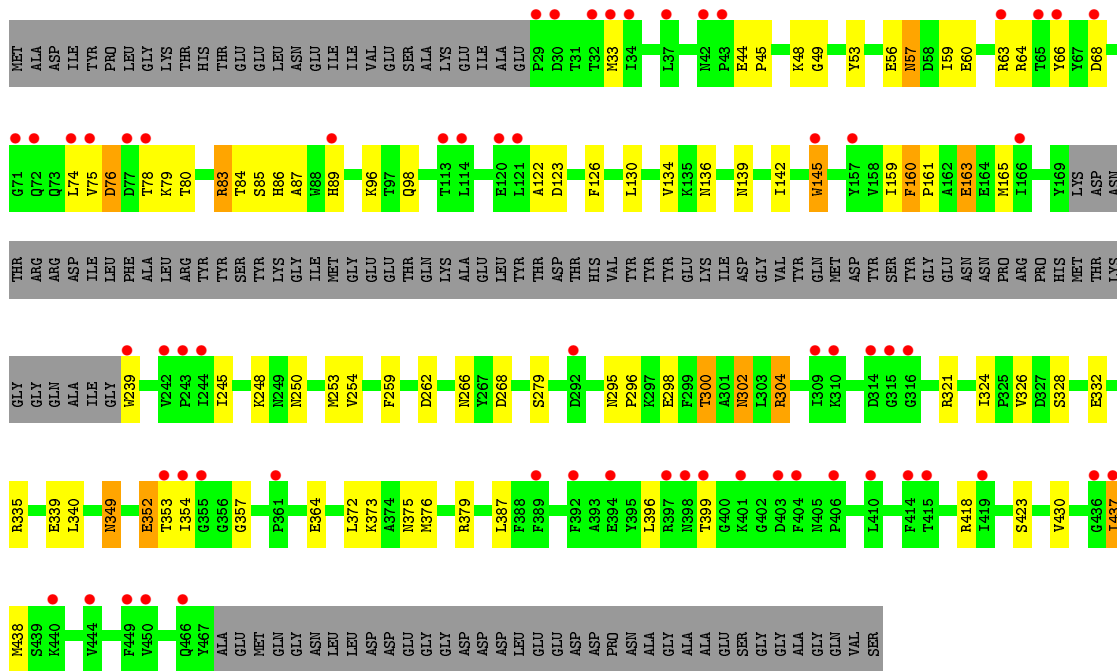


• Molecule 1: PORTAL PROTEIN

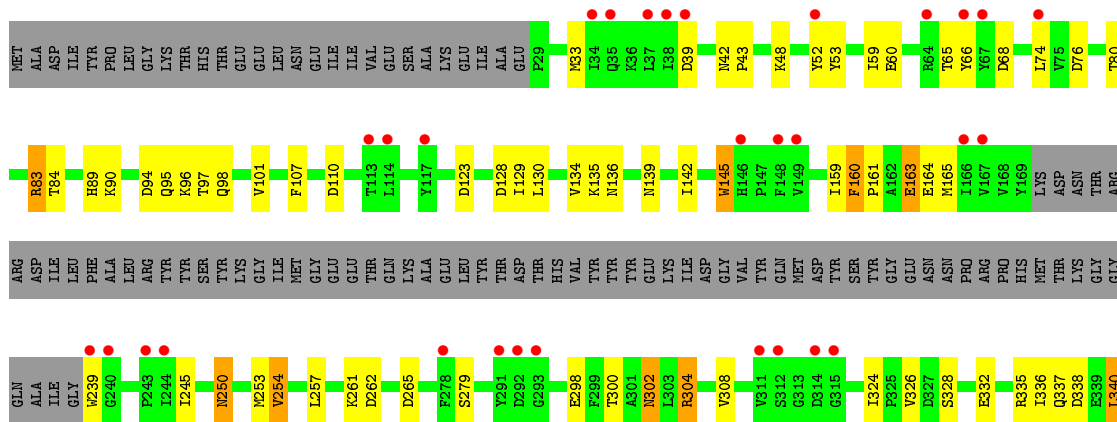


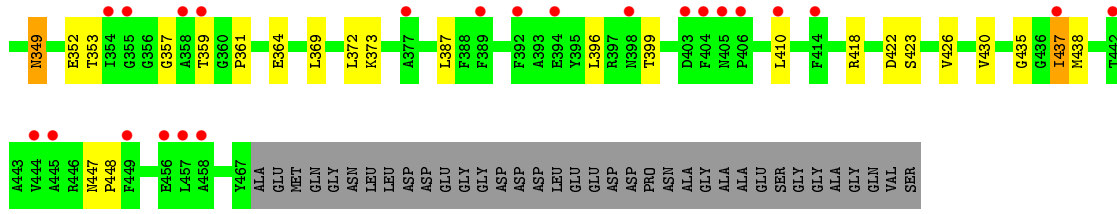


● Molecule 1: PORTAL PROTEIN

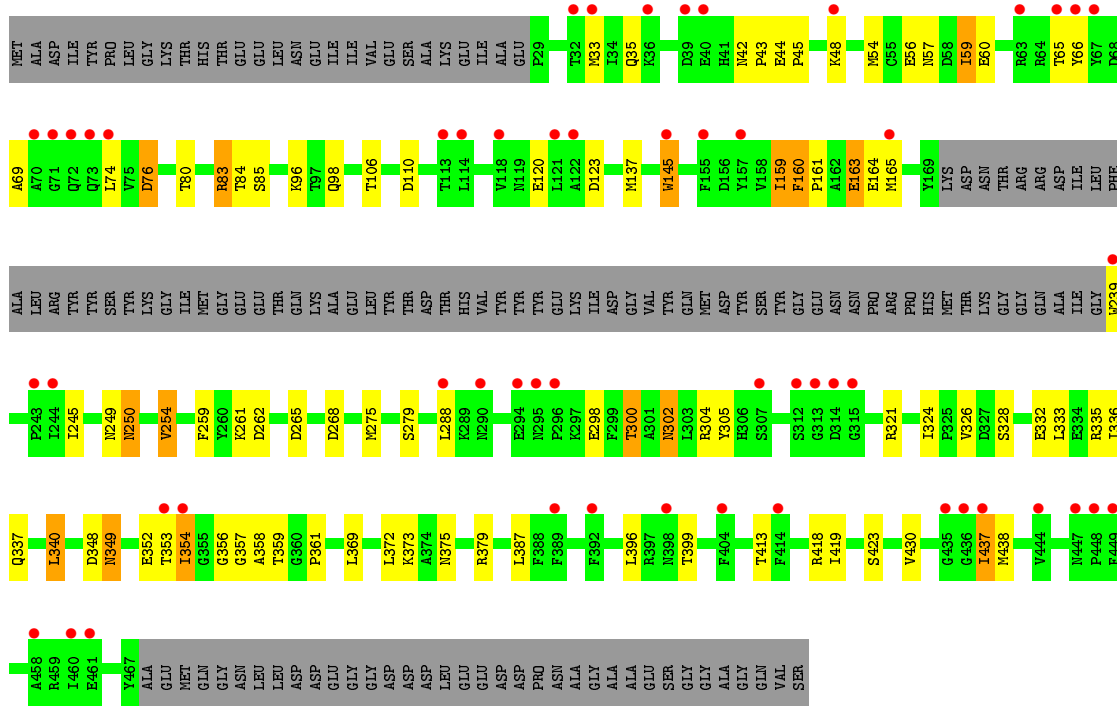


● Molecule 1: PORTAL PROTEIN

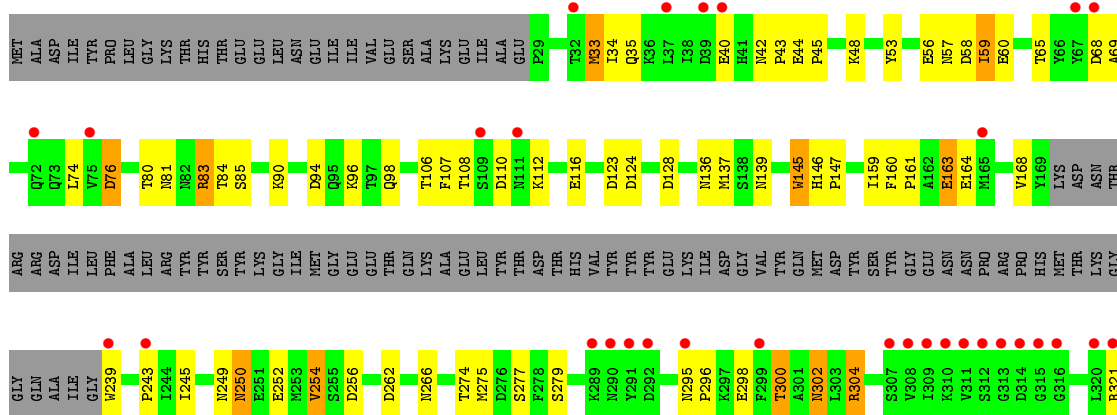


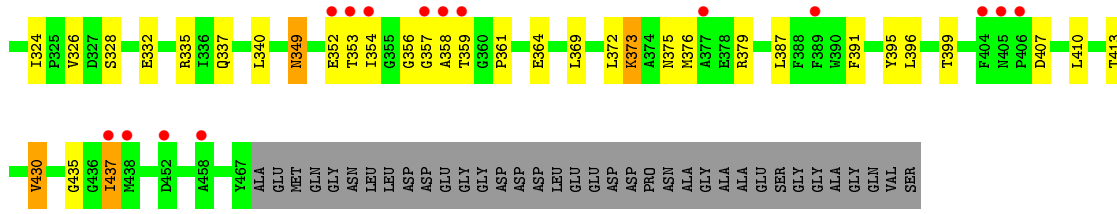


• Molecule 1: PORTAL PROTEIN

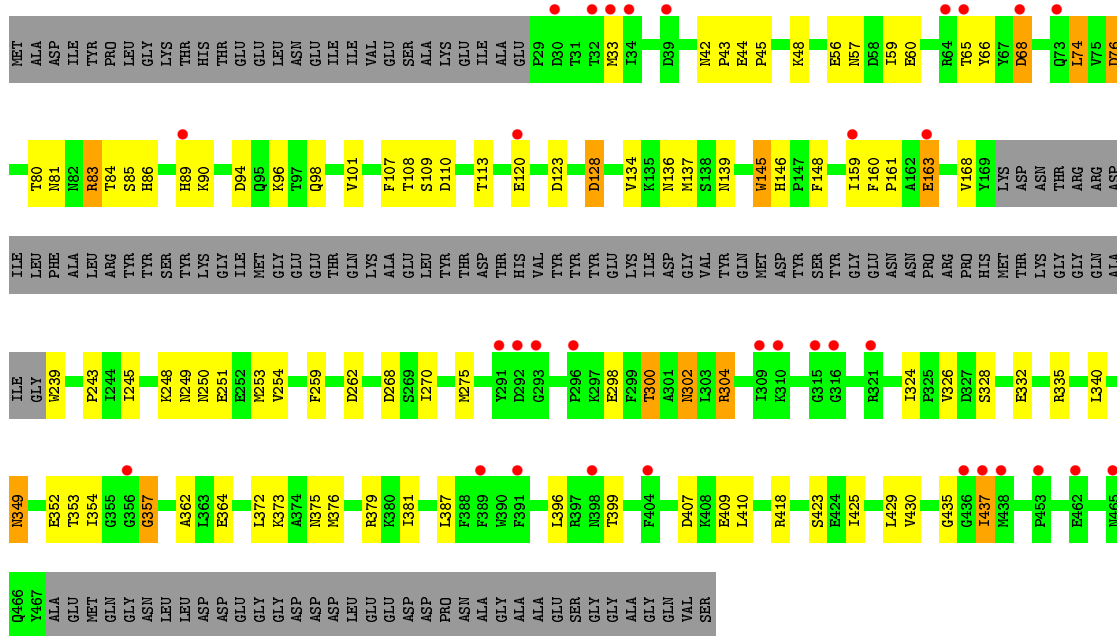


• Molecule 1: PORTAL PROTEIN

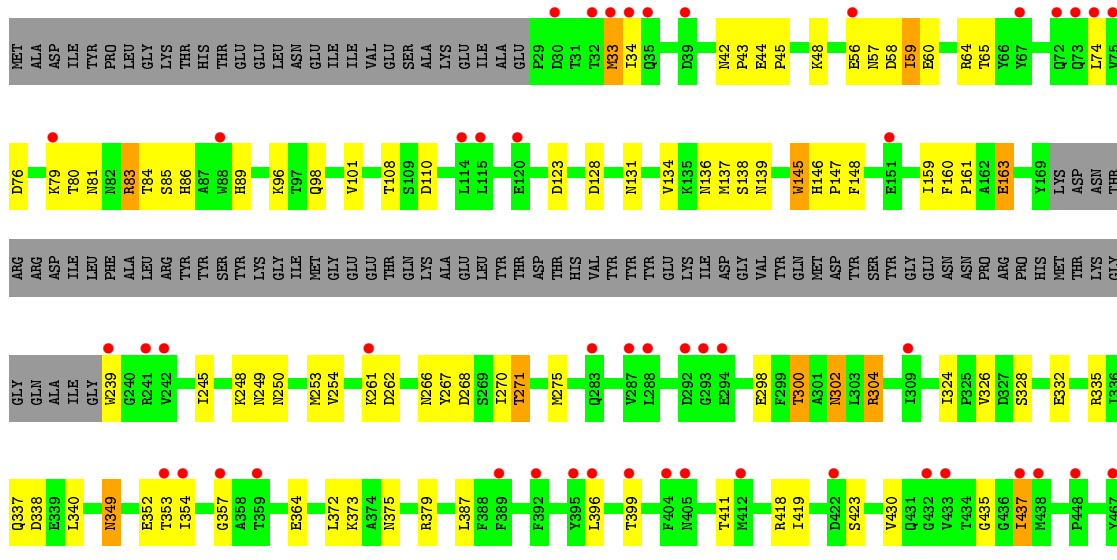




• Molecule 1: PORTAL PROTEIN

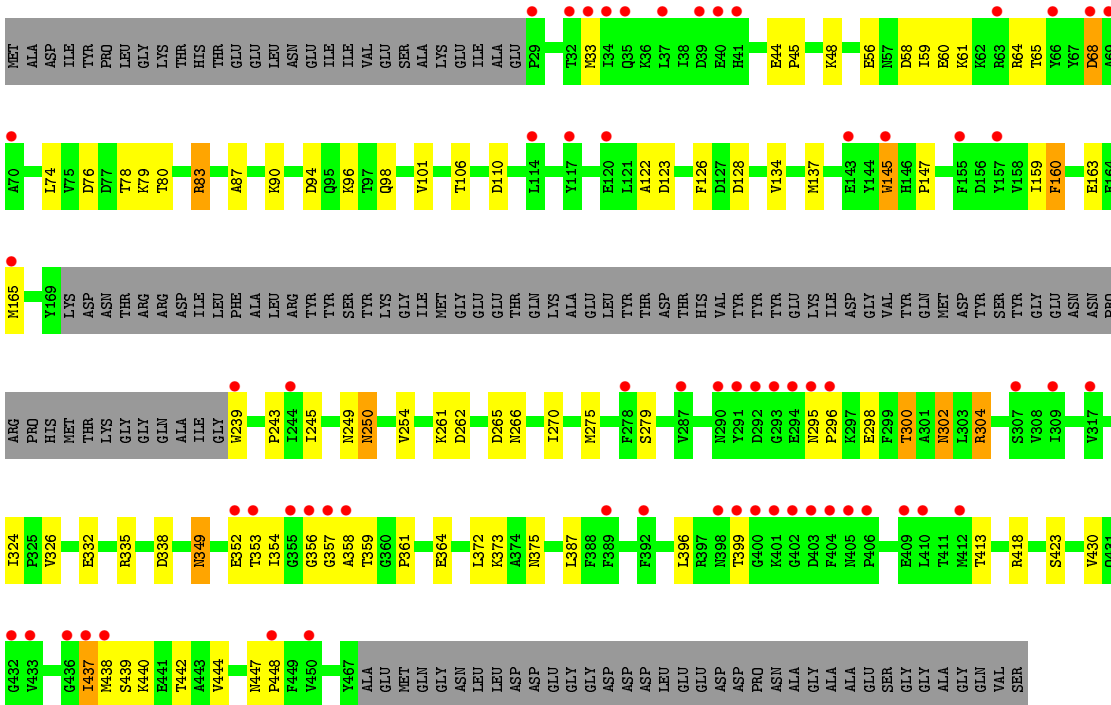


• Molecule 1: PORTAL PROTEIN



ALA
GLU
MET
GLN
GLY
ASN
LEU
LEU
LEU
ASP
ASP
GLU
GLY
GLY
ASP
ASP
ASP
LEU
LEU
LEU
GLU
GLU
GLU
ASP
ASP
PARG
ASN
ALA
GLY
ALA
ALA
GLU
GLU
SER
SER
GLY
GLY
ALA
GLY
GLN
VAL
SER

• Molecule 1: PORTAL PROTEIN



• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN



• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN



• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN



• Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain H:  93% 7%



- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain J:  93% 7%



- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain L:  93% 7%




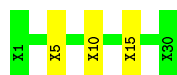
- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain N:  93% 7%




- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain P:  90% 10%



- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain R:  90% 10%



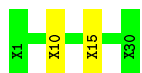
- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain T:  97% 3%



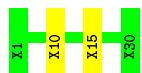
- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain V:  93% 7%



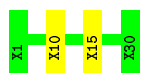
- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain X: 93% 7%



- Molecule 2: UNIDENTIFIED FRAGMENT OF PORTAL PROTEIN

Chain Z: 93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.31Å 221.41Å 421.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 3.40 39.82 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.81-3.40) 99.6 (39.82-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.288 , 0.319 0.280 , 0.310	Depositor DCC
R_{free} test set	1121 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	107.2	Xtrriage
Anisotropy	0.370	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 161.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	39260	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: CA, HG

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	0.42	0/2928	0.55	0/3978
1	C	0.41	0/2928	0.54	0/3978
1	E	0.44	0/2928	0.55	0/3978
1	G	0.44	0/2928	0.57	0/3978
1	I	0.47	0/2928	0.58	0/3978
1	K	0.48	0/2928	0.58	0/3978
1	M	0.46	0/2928	0.58	0/3978
1	O	0.47	0/2928	0.57	0/3978
1	Q	0.53	0/2928	0.62	0/3978
1	S	0.60	0/2928	0.66	0/3978
1	U	0.58	0/2928	0.66	0/3978
1	W	0.49	0/2928	0.60	0/3978
1	Y	0.46	0/2928	0.57	0/3978
All	All	0.48	0/38064	0.59	0/51714

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	2868	0	2686	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2868	0	2686	53	1
1	E	2868	0	2686	46	0
1	G	2868	0	2686	58	0
1	I	2868	0	2686	61	0
1	K	2868	0	2686	57	0
1	M	2868	0	2686	50	0
1	O	2868	0	2685	53	1
1	Q	2868	0	2685	55	0
1	S	2868	0	2686	67	0
1	U	2868	0	2686	68	0
1	W	2868	0	2686	61	0
1	Y	2868	0	2686	51	0
2	B	150	0	36	1	0
2	D	150	0	37	1	0
2	F	150	0	37	1	0
2	H	150	0	38	1	0
2	J	150	0	37	1	0
2	L	150	0	38	1	0
2	N	150	0	36	1	0
2	P	150	0	36	2	0
2	R	150	0	37	2	0
2	T	150	0	37	1	0
2	V	150	0	37	1	0
2	X	150	0	37	1	0
2	Z	150	0	38	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	1	0	0	0	0
3	U	1	0	0	0	0
3	W	1	0	0	0	0
3	Y	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
4	S	1	0	0	0	0
4	U	1	0	0	0	0
4	W	1	0	0	0	0
4	Y	1	0	0	0	0
All	All	39260	0	35397	609	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 8.

The worst 5 of 609 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:M:96:LYS:HD3	1:M:373:LYS:HD3	1.34	1.06
1:S:430:VAL:HG23	1:U:437:ILE:HD11	1.37	1.03
1:C:96:LYS:HD3	1:C:373:LYS:HD3	1.42	1.00
1:Q:96:LYS:HD3	1:Q:373:LYS:HD3	1.46	0.96
1:E:96:LYS:HD3	1:E:373:LYS:HD3	1.48	0.96

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:C:110:ASP:O	1:O:39:ASP:OD2[5_445]	2.08	0.12

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	366/503 (73%)	333 (91%)	31 (8%)	2 (0%)	29	61
1	C	366/503 (73%)	337 (92%)	26 (7%)	3 (1%)	19	51
1	E	366/503 (73%)	338 (92%)	26 (7%)	2 (0%)	29	61
1	G	366/503 (73%)	331 (90%)	33 (9%)	2 (0%)	29	61
1	I	366/503 (73%)	332 (91%)	32 (9%)	2 (0%)	29	61
1	K	366/503 (73%)	339 (93%)	24 (7%)	3 (1%)	19	51
1	M	366/503 (73%)	335 (92%)	29 (8%)	2 (0%)	29	61
1	O	366/503 (73%)	337 (92%)	27 (7%)	2 (0%)	29	61
1	Q	366/503 (73%)	343 (94%)	21 (6%)	2 (0%)	29	61
1	S	366/503 (73%)	333 (91%)	29 (8%)	4 (1%)	14	44
1	U	366/503 (73%)	337 (92%)	26 (7%)	3 (1%)	19	51
1	W	366/503 (73%)	338 (92%)	27 (7%)	1 (0%)	41	72
1	Y	366/503 (73%)	336 (92%)	27 (7%)	3 (1%)	19	51
All	All	4758/6539 (73%)	4369 (92%)	358 (8%)	31 (1%)	22	55

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	357	GLY
1	A	357	GLY
1	C	357	GLY
1	E	357	GLY
1	G	69	ALA

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	296/436 (68%)	270 (91%)	26 (9%)	10	33
1	C	296/436 (68%)	270 (91%)	26 (9%)	10	33
1	E	296/436 (68%)	268 (90%)	28 (10%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	296/436 (68%)	265 (90%)	31 (10%)	7	25
1	I	296/436 (68%)	267 (90%)	29 (10%)	8	28
1	K	296/436 (68%)	265 (90%)	31 (10%)	7	25
1	M	296/436 (68%)	265 (90%)	31 (10%)	7	25
1	O	296/436 (68%)	266 (90%)	30 (10%)	7	27
1	Q	296/436 (68%)	263 (89%)	33 (11%)	6	22
1	S	296/436 (68%)	260 (88%)	36 (12%)	5	18
1	U	296/436 (68%)	265 (90%)	31 (10%)	7	25
1	W	296/436 (68%)	265 (90%)	31 (10%)	7	25
1	Y	296/436 (68%)	269 (91%)	27 (9%)	9	32
All	All	3848/5668 (68%)	3458 (90%)	390 (10%)	7	27

5 of 390 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	68	ASP
1	O	279	SER
1	W	411	THR
1	M	123	ASP
1	M	353	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	73	GLN
1	O	146	HIS
1	W	349	ASN
1	M	86	HIS
1	M	349	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 26 ligands modelled in this entry, 26 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	370/503 (73%)	0.96	61 (16%) 1 2	140, 140, 140, 140	0
1	C	370/503 (73%)	1.10	72 (19%) 1 1	140, 140, 140, 140	0
1	E	370/503 (73%)	1.14	73 (19%) 1 1	140, 140, 140, 140	0
1	G	370/503 (73%)	0.94	67 (18%) 1 1	140, 140, 140, 140	0
1	I	370/503 (73%)	0.95	63 (17%) 1 2	140, 140, 140, 140	0
1	K	370/503 (73%)	0.94	57 (15%) 2 2	140, 140, 140, 140	0
1	M	370/503 (73%)	0.97	61 (16%) 1 2	140, 140, 140, 140	0
1	O	370/503 (73%)	0.85	53 (14%) 2 3	140, 140, 140, 140	0
1	Q	370/503 (73%)	0.87	54 (14%) 2 3	140, 140, 140, 140	0
1	S	370/503 (73%)	0.80	46 (12%) 4 5	140, 140, 140, 140	0
1	U	370/503 (73%)	0.74	33 (8%) 9 11	140, 140, 140, 140	0
1	W	370/503 (73%)	0.74	48 (12%) 3 4	140, 140, 140, 140	0
1	Y	370/503 (73%)	0.96	63 (17%) 1 2	140, 140, 140, 140	0
2	B	0/30	-	-	-	-
2	D	0/30	-	-	-	-
2	F	0/30	-	-	-	-
2	H	0/30	-	-	-	-
2	J	0/30	-	-	-	-
2	L	0/30	-	-	-	-
2	N	0/30	-	-	-	-
2	P	0/30	-	-	-	-
2	R	0/30	-	-	-	-
2	T	0/30	-	-	-	-
2	V	0/30	-	-	-	-
2	X	0/30	-	-	-	-
2	Z	0/30	-	-	-	-
All	All	4810/6929 (69%)	0.92	751 (15%) 2 2	140, 140, 140, 140	0

The worst 5 of 751 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	315	GLY	10.6
1	Y	292	ASP	9.9
1	Y	291	TYR	9.6
1	O	404	PHE	9.0
1	U	291	TYR	8.7

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 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HG	O	701	1/1	0.71	0.14	140,140,140,140	1
4	CA	O	801	1/1	0.72	0.11	140,140,140,140	0
3	HG	S	701	1/1	0.73	0.13	140,140,140,140	1
4	CA	A	801	1/1	0.79	0.10	140,140,140,140	0
4	CA	M	801	1/1	0.82	0.15	140,140,140,140	0
3	HG	M	701	1/1	0.82	0.14	140,140,140,140	1
3	HG	I	701	1/1	0.86	0.12	140,140,140,140	1
4	CA	S	801	1/1	0.87	0.13	140,140,140,140	0
4	CA	C	801	1/1	0.88	0.08	140,140,140,140	0
3	HG	Q	701	1/1	0.88	0.12	140,140,140,140	1
3	HG	C	701	1/1	0.88	0.19	140,140,140,140	1
4	CA	K	801	1/1	0.90	0.12	140,140,140,140	0
4	CA	U	801	1/1	0.91	0.07	140,140,140,140	0
4	CA	Y	801	1/1	0.91	0.07	140,140,140,140	0
3	HG	A	701	1/1	0.92	0.17	140,140,140,140	1
4	CA	I	801	1/1	0.93	0.05	140,140,140,140	0
4	CA	W	801	1/1	0.93	0.17	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	HG	W	701	1/1	0.94	0.09	140,140,140,140	1
3	HG	E	701	1/1	0.95	0.28	140,140,140,140	1
4	CA	Q	801	1/1	0.95	0.08	140,140,140,140	0
3	HG	Y	701	1/1	0.95	0.12	140,140,140,140	1
4	CA	G	801	1/1	0.95	0.12	140,140,140,140	0
3	HG	G	701	1/1	0.96	0.11	140,140,140,140	1
3	HG	K	701	1/1	0.96	0.09	140,140,140,140	1
3	HG	U	701	1/1	0.96	0.10	140,140,140,140	1
4	CA	E	801	1/1	0.97	0.07	140,140,140,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.