



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2024 – 04:23 PM EDT

PDB ID : 3CUE
Title : Crystal structure of a TRAPP subassembly activating the Rab Ypt1p
Authors : Cai, Y.; Reinisch, K.M.
Deposited on : 2008-04-16
Resolution : 3.70 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

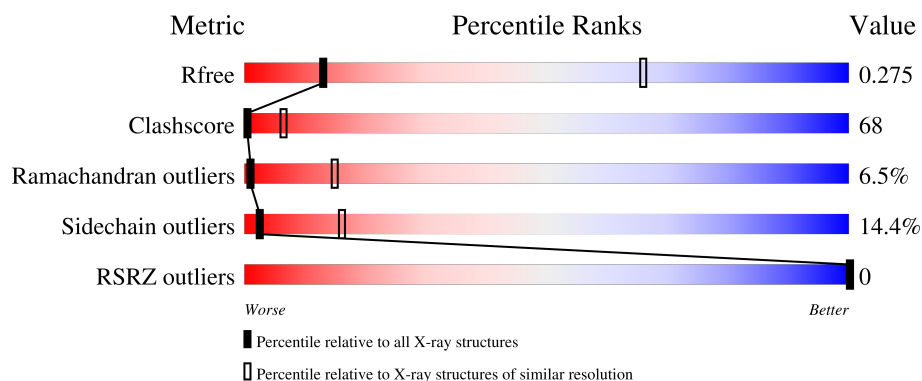
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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.






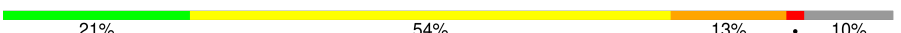
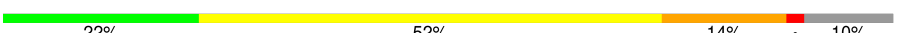
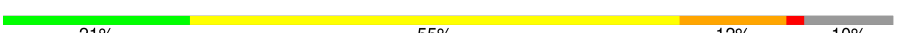
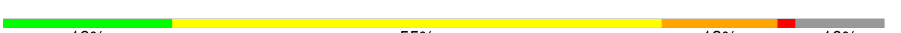




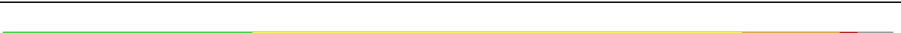

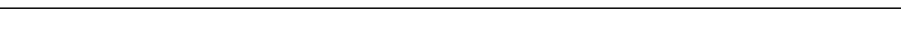

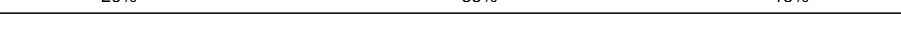
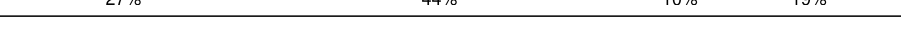
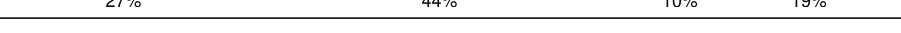
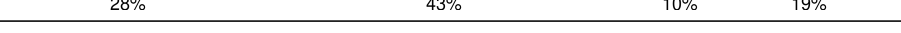
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1017 (3.80-3.60)
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)

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 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	219	<div> <div>17%</div> <div>44%</div> <div>11%</div> <div>27%</div> </div>
1	G	219	<div> <div>15%</div> <div>47%</div> <div>11%</div> <div>27%</div> </div>
1	M	219	<div> <div>16%</div> <div>46%</div> <div>10%</div> <div>27%</div> </div>
1	S	219	<div> <div>17%</div> <div>46%</div> <div>10%</div> <div>27%</div> </div>
2	B	283	<div> <div>18%</div> <div>32%</div> <div>7%</div> <div>41%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	283	
2	N	283	
2	T	283	
3	C	159	
3	I	159	
3	O	159	
3	U	159	
4	D	193	
4	E	193	
4	J	193	
4	K	193	
4	P	193	
4	Q	193	
4	V	193	
4	W	193	
5	F	206	
5	L	206	
5	R	206	
5	X	206	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 32776 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 Transport protein particle 23 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	27	0	0
			1285	833	204	239	9			
1	G	159	Total	C	N	O	S	27	0	0
			1285	833	204	239	9			
1	M	159	Total	C	N	O	S	27	0	0
			1285	833	204	239	9			
1	S	159	Total	C	N	O	S	27	0	0
			1285	833	204	239	9			

- Molecule 2 is a protein called Transport protein particle 31 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	47	0	0
			1359	869	235	246	9			
2	H	167	Total	C	N	O	S	47	0	0
			1359	869	235	246	9			
2	N	167	Total	C	N	O	S	47	0	0
			1359	869	235	246	9			
2	T	167	Total	C	N	O	S	47	0	0
			1359	869	235	246	9			

- Molecule 3 is a protein called Transport protein particle 18 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	143	Total	C	N	O	S	12	0	0
			1190	765	201	217	7			
3	I	143	Total	C	N	O	S	16	0	0
			1190	765	201	217	7			
3	O	143	Total	C	N	O	S	12	0	0
			1190	765	201	217	7			
3	U	143	Total	C	N	O	S	16	0	0
			1190	765	201	217	7			

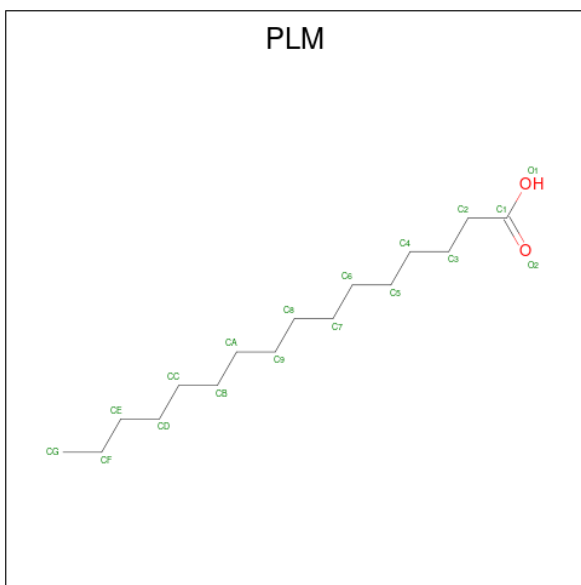
- Molecule 4 is a protein called Transport protein particle 22 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	186	Total	C	N	O	S	28	0	0
			1500	956	246	287	11			
4	E	188	Total	C	N	O	S	1	0	0
			1515	964	249	291	11			
4	J	186	Total	C	N	O	S	28	0	0
			1500	956	246	287	11			
4	K	188	Total	C	N	O	S	1	0	0
			1515	964	249	291	11			
4	P	186	Total	C	N	O	S	28	0	0
			1500	956	246	287	11			
4	Q	188	Total	C	N	O	S	1	0	0
			1515	964	249	291	11			
4	V	186	Total	C	N	O	S	28	0	0
			1500	956	246	287	11			
4	W	188	Total	C	N	O	S	1	0	0
			1515	964	249	291	11			

- Molecule 5 is a protein called GTP-binding protein YPT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	166	Total	C	N	O	S	33	0	0
			1328	848	215	259	6			
5	L	166	Total	C	N	O	S	33	0	0
			1328	848	215	259	6			
5	R	166	Total	C	N	O	S	33	0	0
			1328	848	215	259	6			
5	X	166	Total	C	N	O	S	33	0	0
			1328	848	215	259	6			

- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).

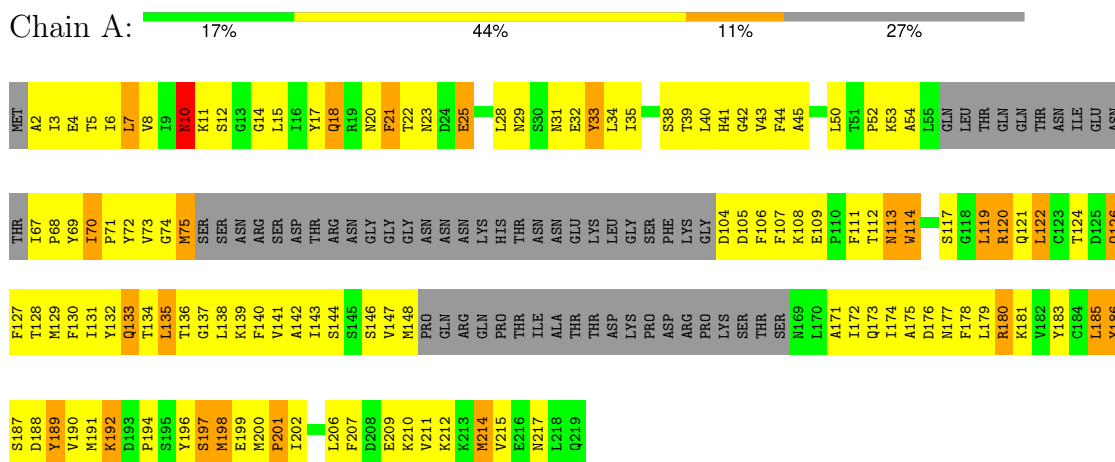


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total 17	C 16	O 1	0	0
6	K	1	Total 17	C 16	O 1	0	0
6	Q	1	Total 17	C 16	O 1	0	0
6	W	1	Total 17	C 16	O 1	0	0

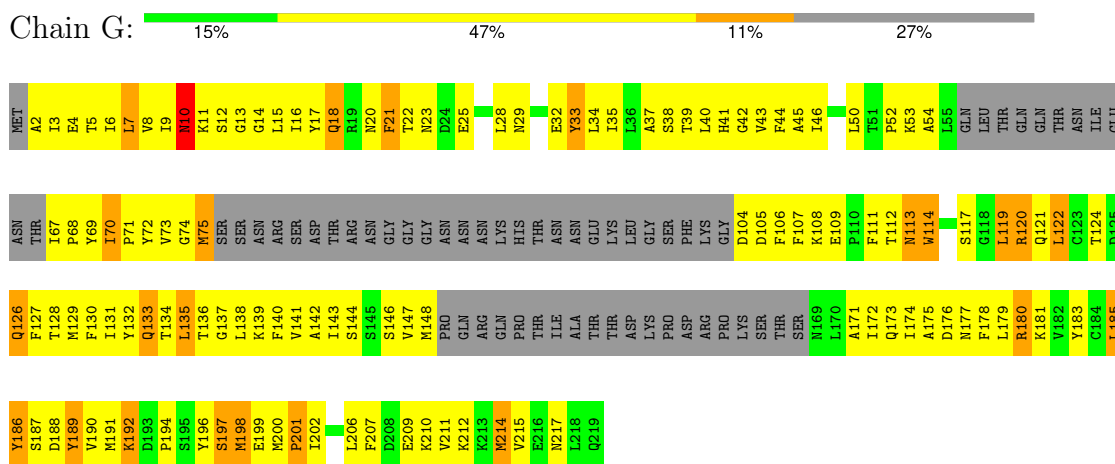
3 Residue-property plots

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.

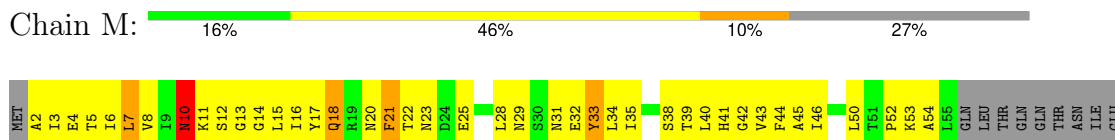
- Molecule 1: Transport protein particle 23 kDa subunit

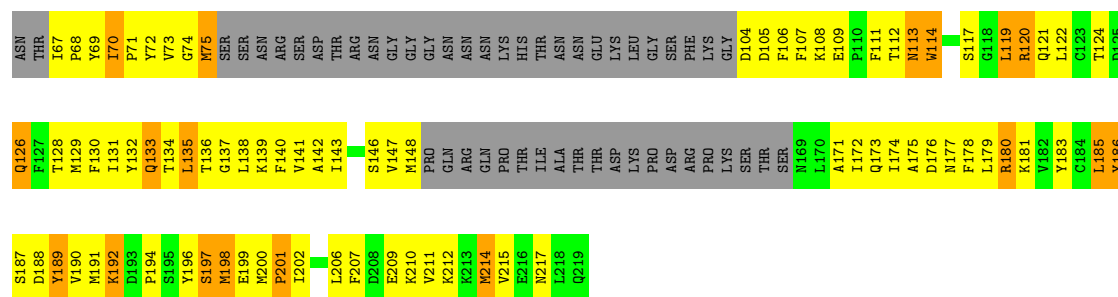


- Molecule 1: Transport protein particle 23 kDa subunit

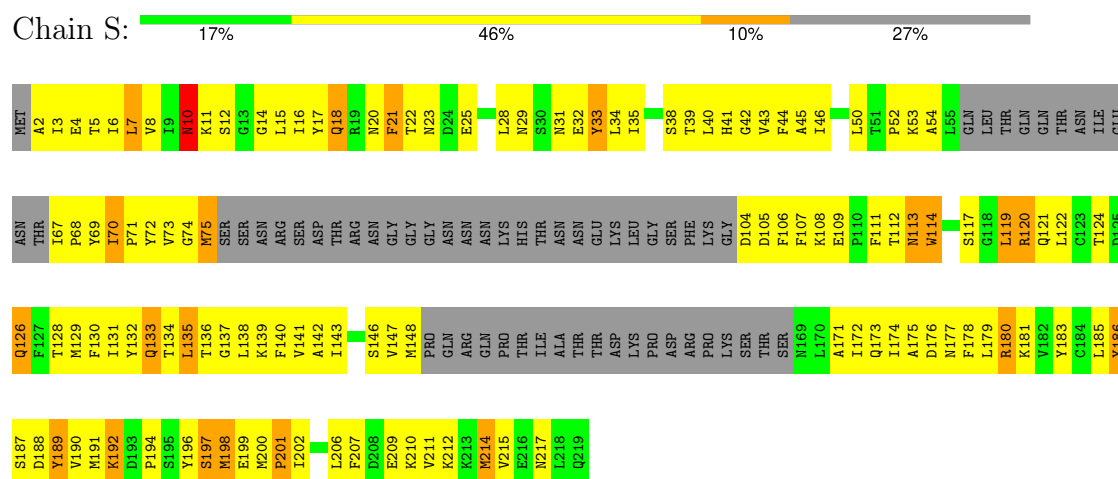


- Molecule 1: Transport protein particle 23 kDa subunit

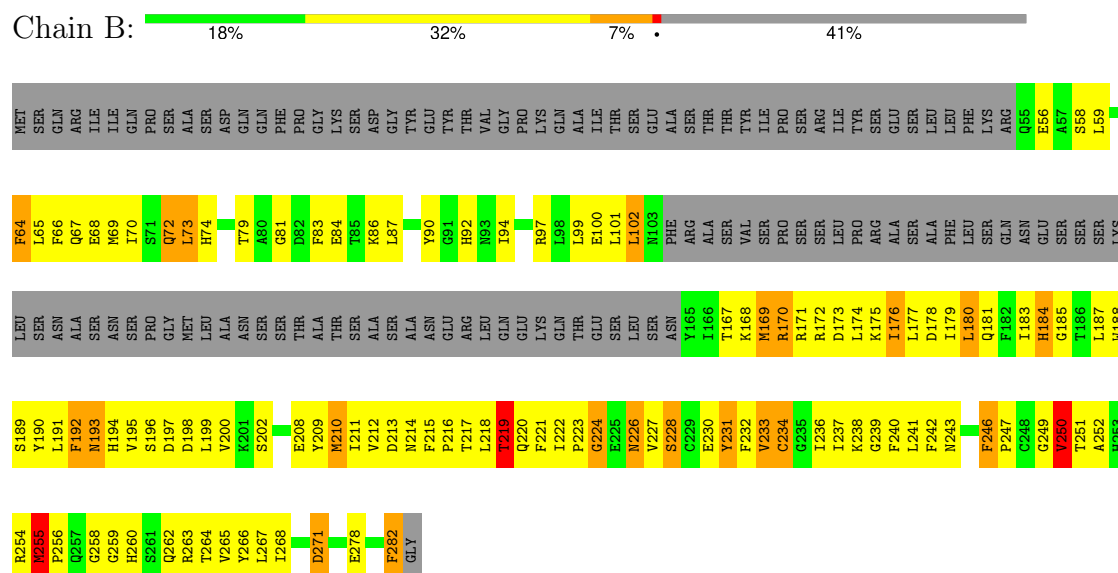




• Molecule 1: Transport protein particle 23 kDa subunit

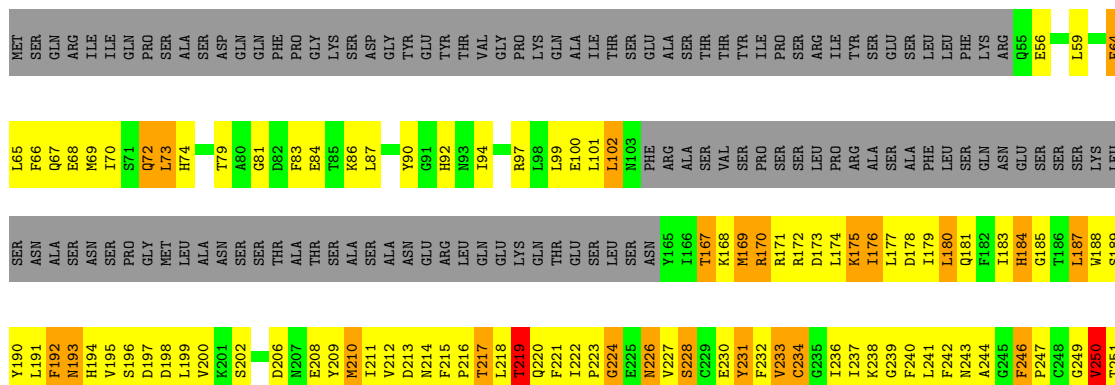


• Molecule 2: Transport protein particle 31 kDa subunit



• Molecule 2: Transport protein particle 31 kDa subunit

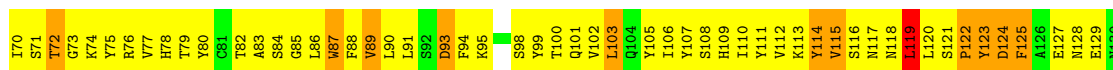
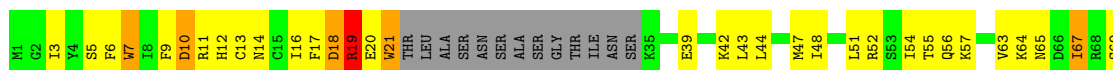






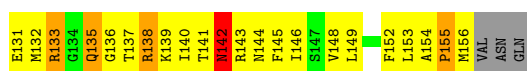
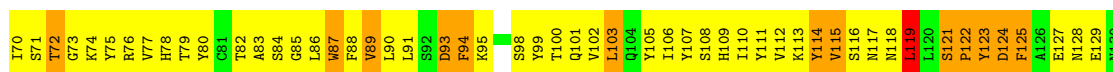
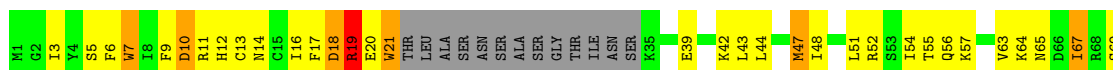
• Molecule 3: Transport protein particle 18 kDa subunit

Chain C: 21% 54% 13% 10%



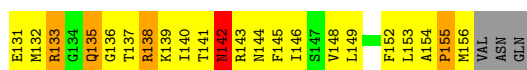
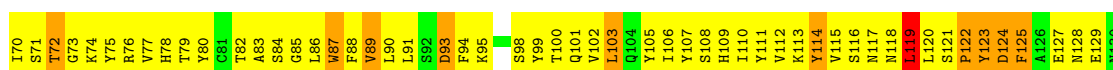
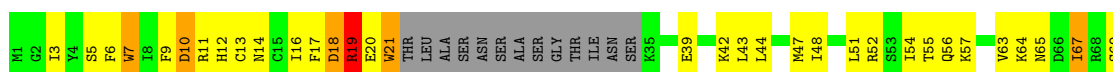
• Molecule 3: Transport protein particle 18 kDa subunit

Chain I: 22% 52% 14% 10%



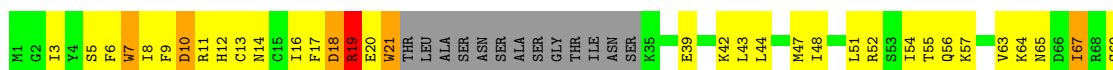
• Molecule 3: Transport protein particle 18 kDa subunit

Chain O: 21% 55% 12% 10%



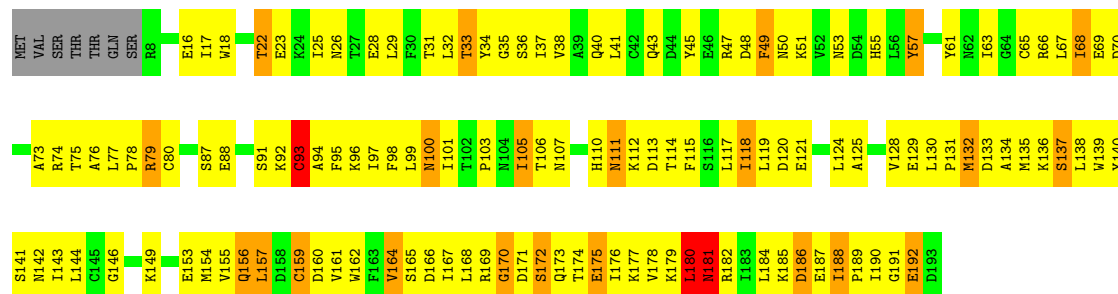
• Molecule 3: Transport protein particle 18 kDa subunit

Chain U: 19% 55% 13% 10%

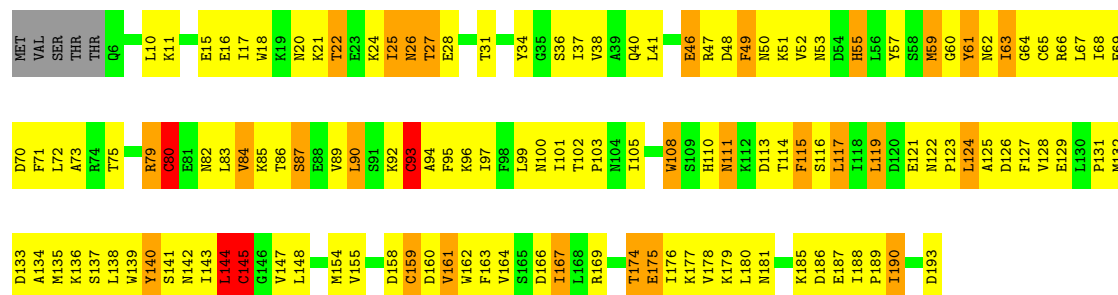




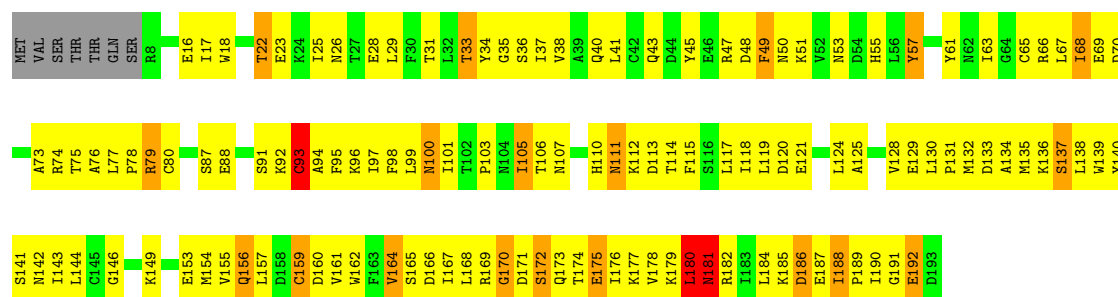
• Molecule 4: Transport protein particle 22 kDa subunit



• Molecule 4: Transport protein particle 22 kDa subunit

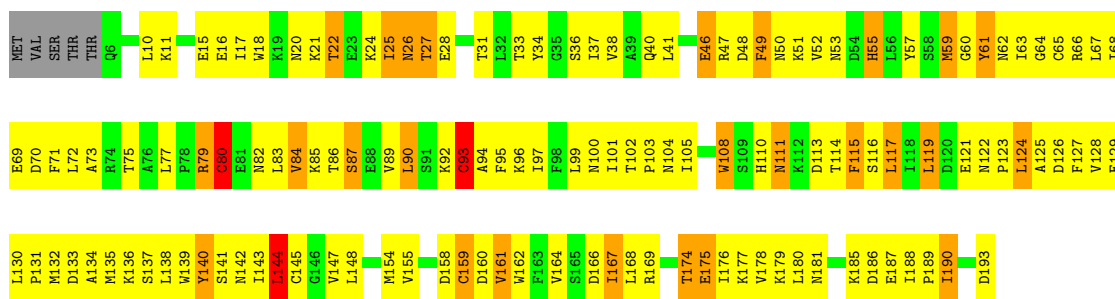


• Molecule 4: Transport protein particle 22 kDa subunit



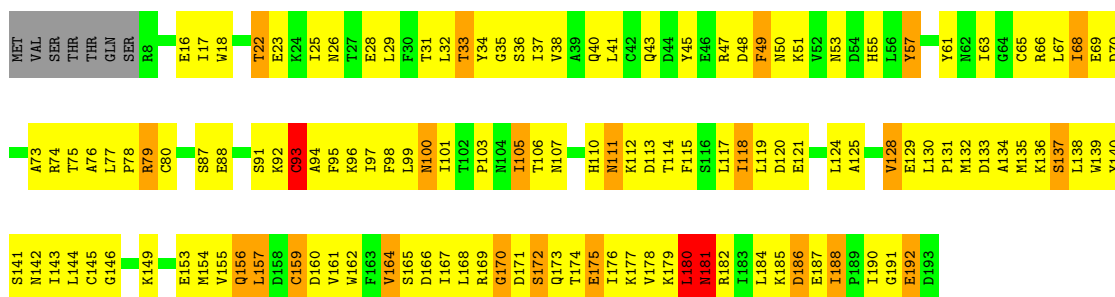
• Molecule 4: Transport protein particle 22 kDa subunit





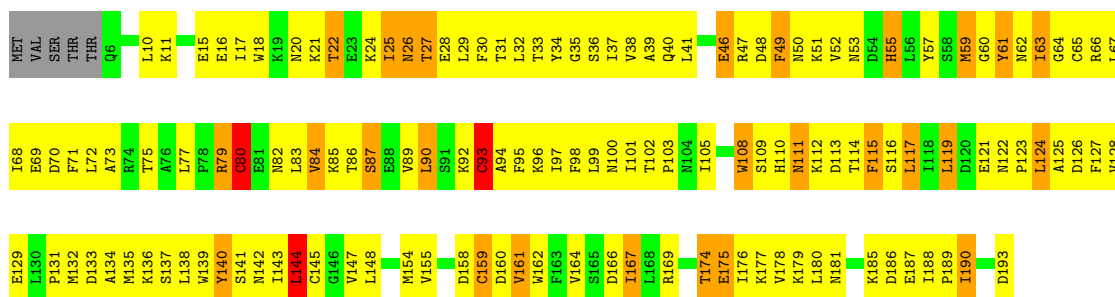
- Molecule 4: Transport protein particle 22 kDa subunit

Chain P: 28% 55% 11%



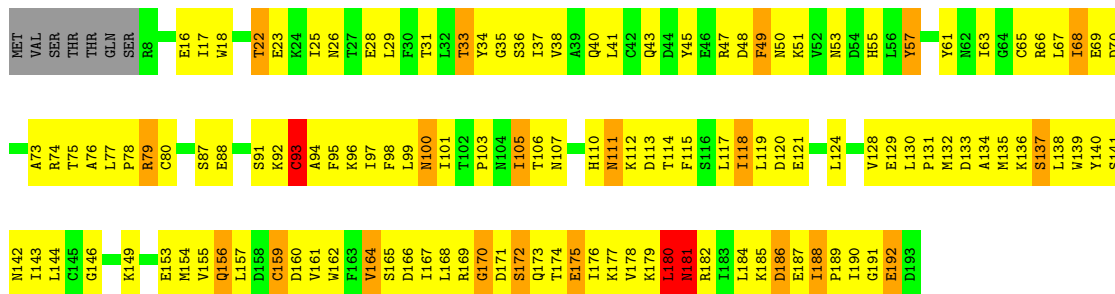
- Molecule 4: Transport protein particle 22 kDa subunit

Chain Q: 25% 57% 14%



- Molecule 4: Transport protein particle 22 kDa subunit

Chain V: 30% 55% 10%



- Molecule 4: Transport protein particle 22 kDa subunit

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.12Å 115.40Å 290.07Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	25.00 – 3.70 25.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (25.00-3.70) 95.8 (25.00-3.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.74Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.265 , 0.299 0.247 , 0.275	Depositor DCC
R_{free} test set	5561 reflections (6.94%)	wwPDB-VP
Wilson B-factor (Å ²)	128.9	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 118.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.387 for -k,-h,-l 0.398 for k,h,-l 0.397 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32776	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: PLM

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	0.67	1/1309 (0.1%)	0.82	0/1764
1	G	0.67	1/1309 (0.1%)	0.82	0/1764
1	M	0.66	1/1309 (0.1%)	0.82	0/1764
1	S	0.67	1/1309 (0.1%)	0.83	0/1764
2	B	0.56	0/1388	0.81	1/1869 (0.1%)
2	H	0.56	0/1388	0.81	1/1869 (0.1%)
2	N	0.55	0/1388	0.82	1/1869 (0.1%)
2	T	0.56	0/1388	0.82	1/1869 (0.1%)
3	C	0.68	1/1218 (0.1%)	0.86	1/1640 (0.1%)
3	I	0.68	1/1218 (0.1%)	0.86	1/1640 (0.1%)
3	O	0.67	1/1218 (0.1%)	0.87	0/1640
3	U	0.67	1/1218 (0.1%)	0.87	1/1640 (0.1%)
4	D	0.59	0/1527	0.83	2/2063 (0.1%)
4	E	0.68	1/1542 (0.1%)	0.93	4/2083 (0.2%)
4	J	0.60	0/1527	0.83	2/2063 (0.1%)
4	K	0.68	0/1542	0.93	4/2083 (0.2%)
4	P	0.60	0/1527	0.83	2/2063 (0.1%)
4	Q	0.69	0/1542	0.93	4/2083 (0.2%)
4	V	0.59	0/1527	0.83	2/2063 (0.1%)
4	W	0.68	0/1542	0.93	4/2083 (0.2%)
5	F	0.59	0/1348	0.92	7/1815 (0.4%)
5	L	0.60	0/1348	0.90	5/1815 (0.3%)
5	R	0.57	0/1348	0.89	5/1815 (0.3%)
5	X	0.59	0/1348	0.90	5/1815 (0.3%)
All	All	0.63	9/33328 (0.0%)	0.86	53/44936 (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
4	D	0	1
4	J	0	1
4	P	0	1
4	V	0	1
All	All	0	4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	109	GLU	CD-OE2	7.58	1.33	1.25
1	G	109	GLU	CD-OE2	7.57	1.33	1.25
1	S	109	GLU	CD-OE2	7.45	1.33	1.25
1	A	109	GLU	CD-OE2	7.31	1.33	1.25
3	U	21	TRP	CB-CG	6.09	1.61	1.50

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	144	LEU	CA-CB-CG	8.62	135.13	115.30
4	W	144	LEU	CA-CB-CG	8.46	134.75	115.30
4	E	144	LEU	CA-CB-CG	8.43	134.69	115.30
4	Q	144	LEU	CA-CB-CG	8.35	134.50	115.30
5	F	67	GLN	C-N-CA	-7.59	102.72	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	57	TYR	Sidechain
4	J	57	TYR	Sidechain
4	P	57	TYR	Sidechain
4	V	57	TYR	Sidechain

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1285	0	1290	216	0
1	G	1285	0	1290	225	0
1	M	1285	0	1290	218	0
1	S	1285	0	1290	218	0
2	B	1359	0	1335	166	0
2	H	1359	0	1335	173	0
2	N	1359	0	1335	169	0
2	T	1359	0	1335	172	0
3	C	1190	0	1166	213	0
3	I	1190	0	1166	220	0
3	O	1190	0	1166	213	0
3	U	1190	0	1166	228	0
4	D	1500	0	1500	211	0
4	E	1515	0	1512	179	0
4	J	1500	0	1500	209	0
4	K	1515	0	1512	187	0
4	P	1500	0	1500	209	0
4	Q	1515	0	1512	200	0
4	V	1500	0	1500	209	0
4	W	1515	0	1512	203	0
5	F	1328	0	1329	178	0
5	L	1328	0	1329	181	0
5	R	1328	0	1329	175	0
5	X	1328	0	1329	182	0
6	E	17	0	31	6	0
6	K	17	0	31	5	0
6	Q	17	0	31	7	0
6	W	17	0	31	6	0
All	All	32776	0	32652	4335	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 68.

The worst 5 of 4335 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)
4:D:79:ARG:HH21	4:D:190:ILE:HD12	1.04	1.17
4:P:79:ARG:HH21	4:P:190:ILE:HD12	1.01	1.17
3:C:39:GLU:HA	3:C:42:LYS:HE2	1.22	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:68:GLU:HG2	5:L:69:ARG:H	1.09	1.16
4:V:79:ARG:HH21	4:V:190:ILE:HD12	1.02	1.16

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	151/219 (69%)	123 (82%)	21 (14%)	7 (5%)	2	19
1	G	151/219 (69%)	124 (82%)	21 (14%)	6 (4%)	2	22
1	M	151/219 (69%)	124 (82%)	21 (14%)	6 (4%)	2	22
1	S	151/219 (69%)	124 (82%)	21 (14%)	6 (4%)	2	22
2	B	163/283 (58%)	126 (77%)	25 (15%)	12 (7%)	1	12
2	H	163/283 (58%)	126 (77%)	25 (15%)	12 (7%)	1	12
2	N	163/283 (58%)	126 (77%)	24 (15%)	13 (8%)	1	10
2	T	163/283 (58%)	126 (77%)	23 (14%)	14 (9%)	0	9
3	C	139/159 (87%)	107 (77%)	20 (14%)	12 (9%)	0	9
3	I	139/159 (87%)	107 (77%)	20 (14%)	12 (9%)	0	9
3	O	139/159 (87%)	107 (77%)	20 (14%)	12 (9%)	0	9
3	U	139/159 (87%)	106 (76%)	21 (15%)	12 (9%)	0	9
4	D	184/193 (95%)	147 (80%)	22 (12%)	15 (8%)	1	9
4	E	186/193 (96%)	148 (80%)	28 (15%)	10 (5%)	1	17
4	J	184/193 (95%)	146 (79%)	24 (13%)	14 (8%)	1	11
4	K	186/193 (96%)	149 (80%)	27 (14%)	10 (5%)	1	17
4	P	184/193 (95%)	147 (80%)	21 (11%)	16 (9%)	0	9
4	Q	186/193 (96%)	148 (80%)	28 (15%)	10 (5%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	V	184/193 (95%)	146 (79%)	23 (12%)	15 (8%)	1	9
4	W	186/193 (96%)	147 (79%)	29 (16%)	10 (5%)	1	17
5	F	162/206 (79%)	122 (75%)	32 (20%)	8 (5%)	2	18
5	L	162/206 (79%)	122 (75%)	32 (20%)	8 (5%)	2	18
5	R	162/206 (79%)	122 (75%)	32 (20%)	8 (5%)	2	18
5	X	162/206 (79%)	122 (75%)	32 (20%)	8 (5%)	2	18
All	All	3940/5012 (79%)	3092 (78%)	592 (15%)	256 (6%)	1	15

5 of 256 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	MET
2	B	171	ARG
2	B	224	GLY
3	C	10	ASP
3	C	124	ASP

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	145/199 (73%)	120 (83%)	25 (17%)	1	11
1	G	145/199 (73%)	120 (83%)	25 (17%)	1	11
1	M	145/199 (73%)	120 (83%)	25 (17%)	1	11
1	S	145/199 (73%)	121 (83%)	24 (17%)	2	12
2	B	149/249 (60%)	123 (83%)	26 (17%)	1	10
2	H	149/249 (60%)	124 (83%)	25 (17%)	1	11
2	N	149/249 (60%)	124 (83%)	25 (17%)	1	11
2	T	149/249 (60%)	123 (83%)	26 (17%)	1	10
3	C	132/145 (91%)	114 (86%)	18 (14%)	3	18
3	I	132/145 (91%)	114 (86%)	18 (14%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	132/145 (91%)	114 (86%)	18 (14%)	3	18
3	U	132/145 (91%)	114 (86%)	18 (14%)	3	18
4	D	171/178 (96%)	151 (88%)	20 (12%)	4	22
4	E	173/178 (97%)	143 (83%)	30 (17%)	1	10
4	J	171/178 (96%)	151 (88%)	20 (12%)	4	22
4	K	173/178 (97%)	143 (83%)	30 (17%)	1	10
4	P	171/178 (96%)	151 (88%)	20 (12%)	4	22
4	Q	173/178 (97%)	142 (82%)	31 (18%)	1	9
4	V	171/178 (96%)	151 (88%)	20 (12%)	4	22
4	W	173/178 (97%)	142 (82%)	31 (18%)	1	9
5	F	148/183 (81%)	135 (91%)	13 (9%)	8	32
5	L	148/183 (81%)	135 (91%)	13 (9%)	8	32
5	R	148/183 (81%)	135 (91%)	13 (9%)	8	32
5	X	148/183 (81%)	135 (91%)	13 (9%)	8	32
All	All	3672/4528 (81%)	3145 (86%)	527 (14%)	2	16

5 of 527 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	V	16	GLU
4	V	157	LEU
3	U	142	ASN
5	X	77	TYR
3	I	114	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	173	GLN
5	X	121	ASN
4	P	100	ASN
5	X	97	ASN
4	V	55	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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
6	PLM	W	194	4	16,16,17	1.15	1 (6%)	15,15,17	1.37	3 (20%)
6	PLM	K	194	4	16,16,17	1.13	1 (6%)	15,15,17	1.38	4 (26%)
6	PLM	Q	194	4	16,16,17	1.14	1 (6%)	15,15,17	1.38	4 (26%)
6	PLM	E	194	4	16,16,17	1.12	1 (6%)	15,15,17	1.37	3 (20%)

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
6	PLM	W	194	4	-	1/14/14/15	-
6	PLM	K	194	4	-	1/14/14/15	-
6	PLM	Q	194	4	-	1/14/14/15	-
6	PLM	E	194	4	-	1/14/14/15	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	194	PLM	O1-C1	-4.41	1.19	1.42
6	Q	194	PLM	O1-C1	-4.39	1.19	1.42
6	K	194	PLM	O1-C1	-4.34	1.20	1.42
6	E	194	PLM	O1-C1	-4.31	1.20	1.42

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	194	PLM	C9-C8-C7	-2.53	101.60	114.37
6	Q	194	PLM	C9-C8-C7	-2.48	101.86	114.37
6	K	194	PLM	C9-C8-C7	-2.47	101.88	114.37
6	W	194	PLM	C9-C8-C7	-2.42	102.15	114.37
6	Q	194	PLM	CC-CB-CA	-2.21	103.22	114.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	194	PLM	O1-C1-C2-C3
6	K	194	PLM	O1-C1-C2-C3
6	Q	194	PLM	O1-C1-C2-C3
6	W	194	PLM	O1-C1-C2-C3

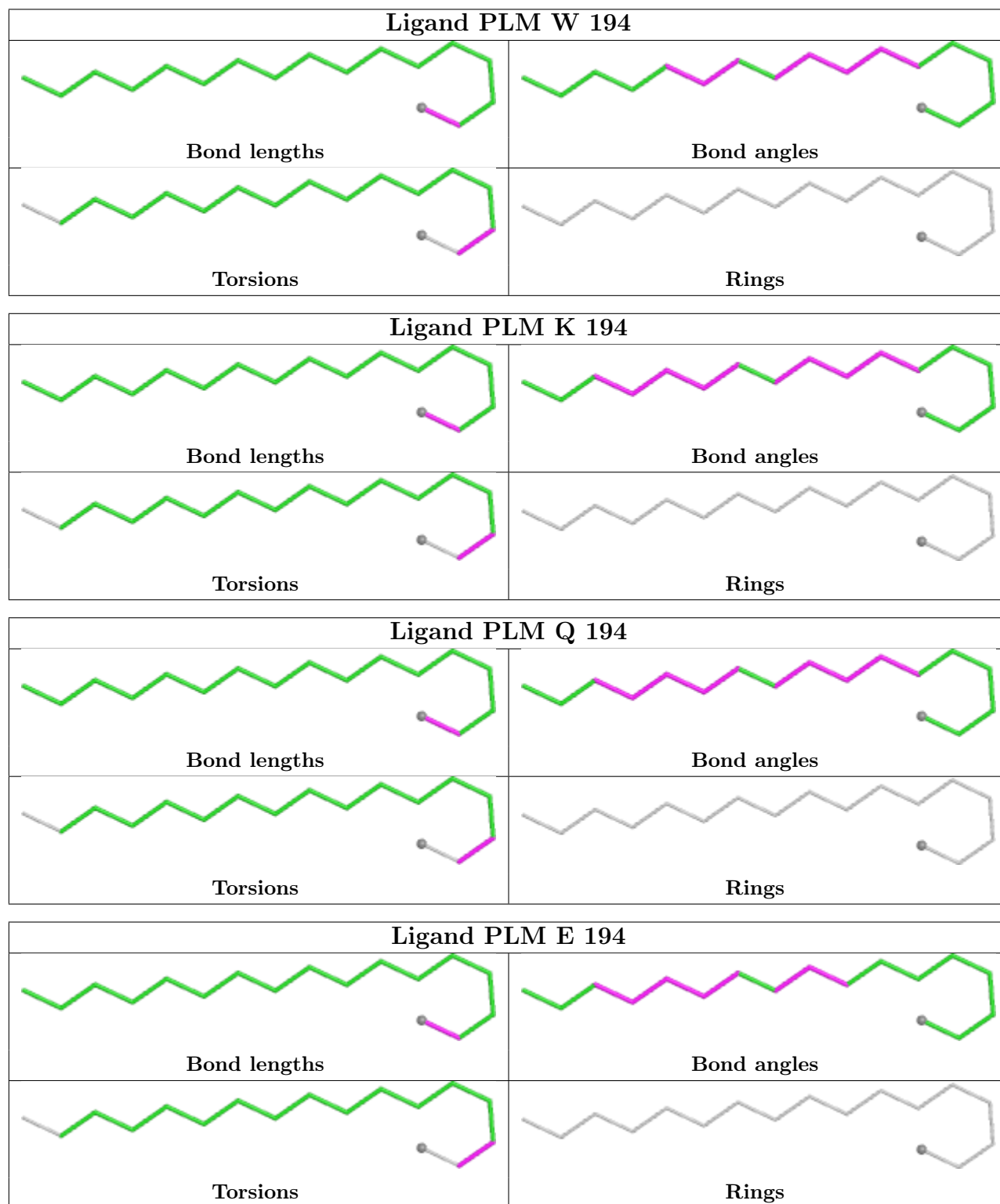
There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	W	194	PLM	6	0
6	K	194	PLM	5	0
6	Q	194	PLM	7	0
6	E	194	PLM	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	159/219 (72%)	-1.51	0 100 100	54, 111, 158, 168	6 (3%)
1	G	159/219 (72%)	-1.51	0 100 100	56, 114, 159, 167	6 (3%)
1	M	159/219 (72%)	-1.52	0 100 100	55, 112, 158, 168	6 (3%)
1	S	159/219 (72%)	-1.57	0 100 100	55, 112, 159, 168	6 (3%)
2	B	167/283 (59%)	-1.51	0 100 100	58, 128, 172, 188	10 (5%)
2	H	167/283 (59%)	-1.56	0 100 100	57, 128, 171, 192	10 (5%)
2	N	167/283 (59%)	-1.51	0 100 100	57, 128, 171, 189	10 (5%)
2	T	167/283 (59%)	-1.57	0 100 100	58, 126, 172, 192	10 (5%)
3	C	143/159 (89%)	-1.52	0 100 100	41, 116, 155, 171	2 (1%)
3	I	143/159 (89%)	-1.58	0 100 100	43, 117, 155, 175	3 (2%)
3	O	143/159 (89%)	-1.59	0 100 100	42, 117, 156, 174	2 (1%)
3	U	143/159 (89%)	-1.57	0 100 100	41, 116, 152, 171	3 (2%)
4	D	186/193 (96%)	-1.55	0 100 100	56, 132, 168, 185	7 (3%)
4	E	188/193 (97%)	-1.52	0 100 100	79, 110, 140, 183	1 (0%)
4	J	186/193 (96%)	-1.53	0 100 100	56, 133, 167, 186	7 (3%)
4	K	188/193 (97%)	-1.57	0 100 100	79, 111, 140, 183	1 (0%)
4	P	186/193 (96%)	-1.54	0 100 100	57, 132, 168, 186	7 (3%)
4	Q	188/193 (97%)	-1.51	0 100 100	78, 110, 141, 184	1 (0%)
4	V	186/193 (96%)	-1.58	0 100 100	56, 132, 167, 185	7 (3%)
4	W	188/193 (97%)	-1.57	0 100 100	79, 111, 140, 182	1 (0%)
5	F	166/206 (80%)	-1.51	0 100 100	57, 145, 172, 178	7 (4%)
5	L	166/206 (80%)	-1.49	0 100 100	57, 146, 173, 179	7 (4%)
5	R	166/206 (80%)	-1.45	0 100 100	56, 146, 171, 175	7 (4%)
5	X	166/206 (80%)	-1.55	0 100 100	57, 146, 171, 176	7 (4%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4036/5012 (80%)	-1.54	0 100 100	41, 123, 169, 192	134 (3%)

There are no RSRZ outliers to report.

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 monosaccharides in this entry.

6.4 Ligands [i](#)

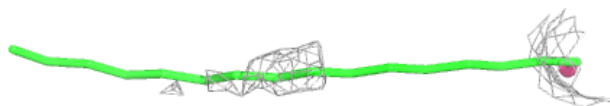
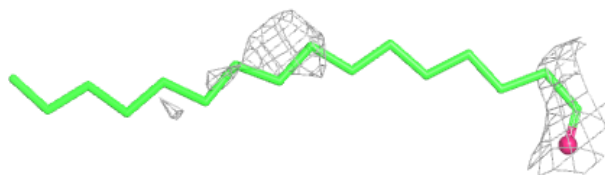
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PLM	E	194	17/18	0.99	0.07	102,105,111,111	0
6	PLM	K	194	17/18	0.99	0.08	104,106,113,114	0
6	PLM	Q	194	17/18	0.99	0.09	100,103,111,112	0
6	PLM	W	194	17/18	0.99	0.08	107,108,111,111	0

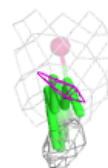
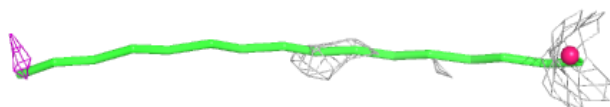
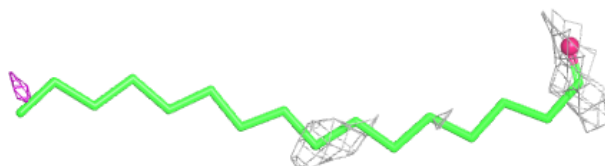
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PLM E 194:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

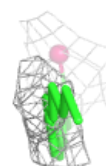
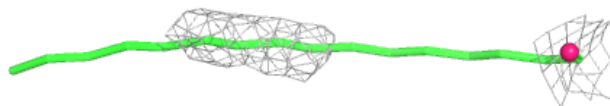
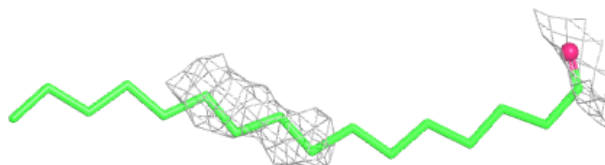
**Electron density around PLM K 194:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

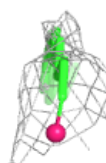
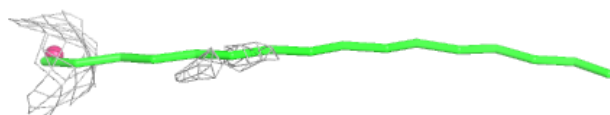
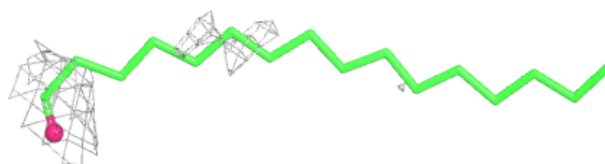


Electron density around PLM Q 194:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PLM W 194:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.