wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 11:57 pm GMT

PDB ID	:	5FQ6
Title	:	Crystal structure of the SusCD complex BT2261-2264 from Bacteroides thetaiotaomicron
Authors	:	Glenwright, A.J.; Pothula, K.R.; Chorev, D.S.; Basle, A.; Robinson, C.V.; Kleinekathoefer, U.; Bolam, D.N.; van den Berg, B.
Deposited on	:	2015-12-07
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

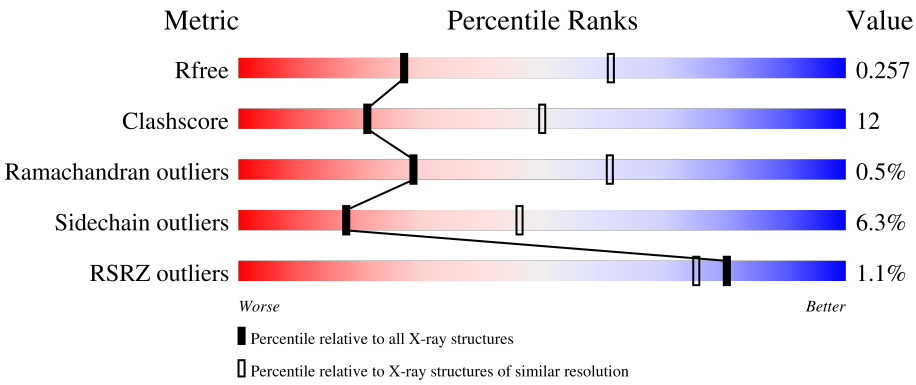
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	480	72% 26% •
1	C	480	77% 22% •
1	H	480	% 70% 26% •
1	L	480	% 61% 35% •

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Mol	Chain	Length	Quality of chain
2	B	984	.% 66% 27%
2	D	984	.% 72% 21%
2	I	984	.% 71% 23%
2	M	984	.% 71% 23%
3	E	148	.% 80% 17%
3	F	148	5% 70% 28%
3	J	148	2% 70% 26%
3	N	148	6% 62% 34%
4	G	10	10% 80% 20%
4	K	10	80% 20%
4	O	10	10% 60% 40%
4	P	10	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 49282 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 PUTATIVE LIPOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	480	3749	2373	616	743	17	0	1	0
1	C	480	3749	2373	616	743	17	0	1	0
1	H	480	3749	2373	616	743	17	0	1	0
1	L	480	3749	2373	616	743	17	0	1	0

- Molecule 2 is a protein called SUSC/RAGA FAMILY TONB-LINKED OUTER MEMBRANE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	941	7326	4635	1222	1439	30	0	0	0
2	D	945	7359	4658	1226	1445	30	0	0	0
2	I	947	7374	4665	1230	1449	30	0	0	0
2	M	948	7383	4670	1231	1452	30	0	0	0

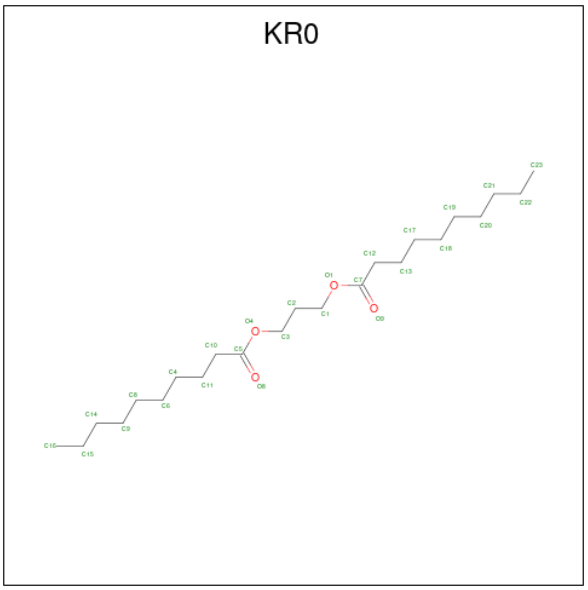
- Molecule 3 is a protein called UNCHARACTERIZED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	146	1142	721	180	236	5	0	0	0
3	F	146	1142	721	180	236	5	0	0	0
3	J	146	1142	721	180	236	5	0	0	0
3	N	146	1142	721	180	236	5	0	0	0

- Molecule 4 is a protein called BT_2261.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	10	40	20	10	10	0	0	0
4	K	10	40	20	10	10	0	0	0
4	O	10	40	20	10	10	0	0	0
4	P	10	40	20	10	10	0	0	0

- Molecule 5 is 3-decanoyloxypropyl decanoate (three-letter code: KR0) (formula: $C_{23}H_{44}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	27	23	4	0	0
5	D	1	27	23	4	0	0
5	I	1	27	23	4	0	0
5	M	1	27	23	4	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	B	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Na 1 1	0	0
6	I	1	Total Na 1 1	0	0
6	M	1	Total Na 1 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

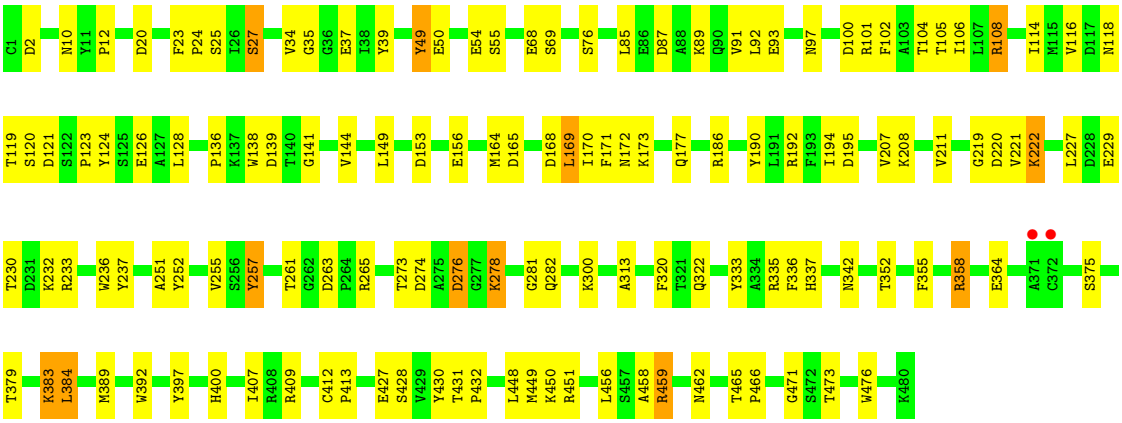
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	D	1	Total Ca 1 1	0	0
7	I	1	Total Ca 1 1	0	0
7	M	1	Total Ca 1 1	0	0

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.

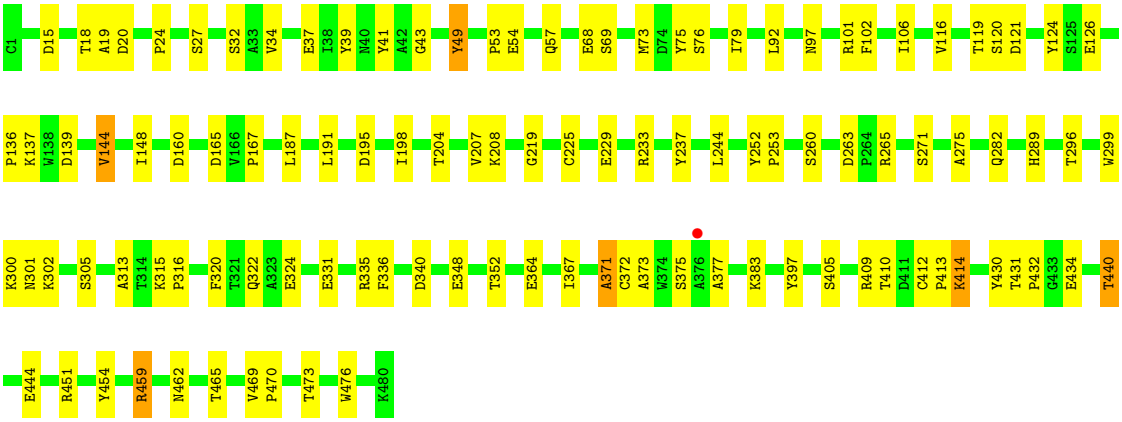
• Molecule 1: PUTATIVE LIPOPROTEIN

Chain A: 72% 26%



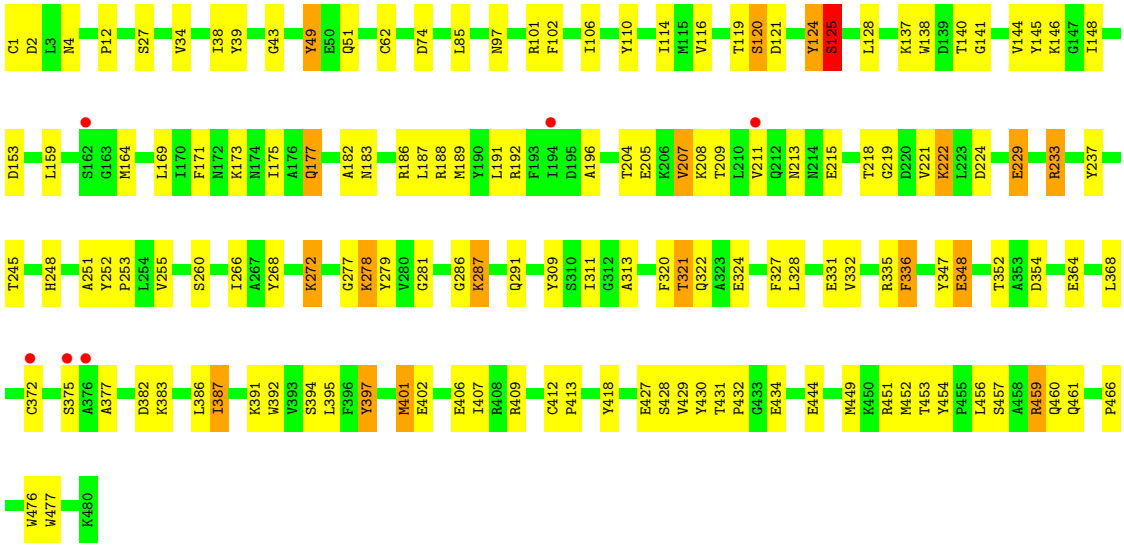
• Molecule 1: PUTATIVE LIPOPROTEIN

Chain C: 77% 22%



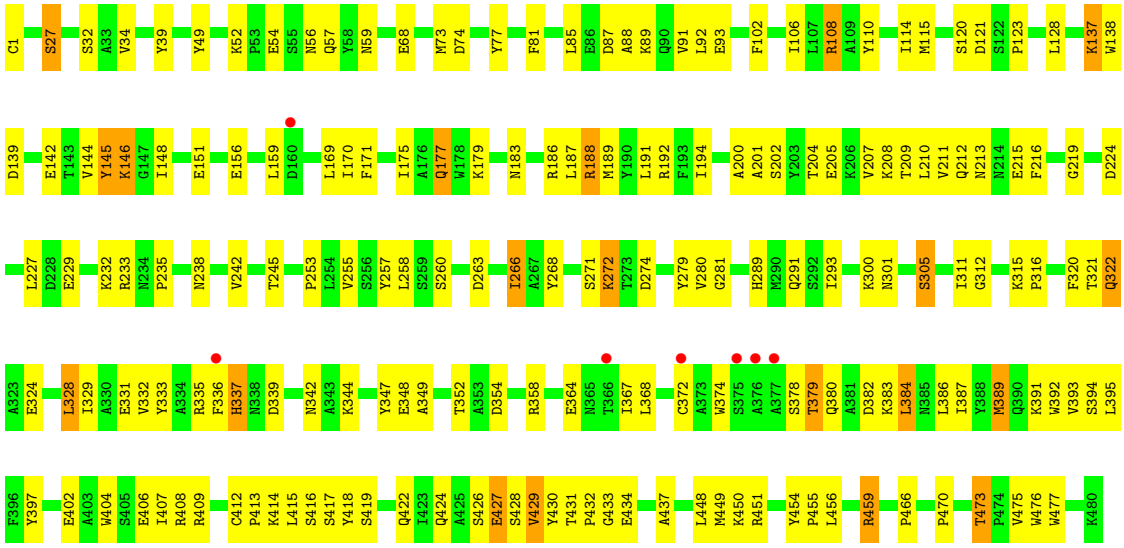
• Molecule 1: PUTATIVE LIPOPROTEIN

Chain H: % 70% 26%



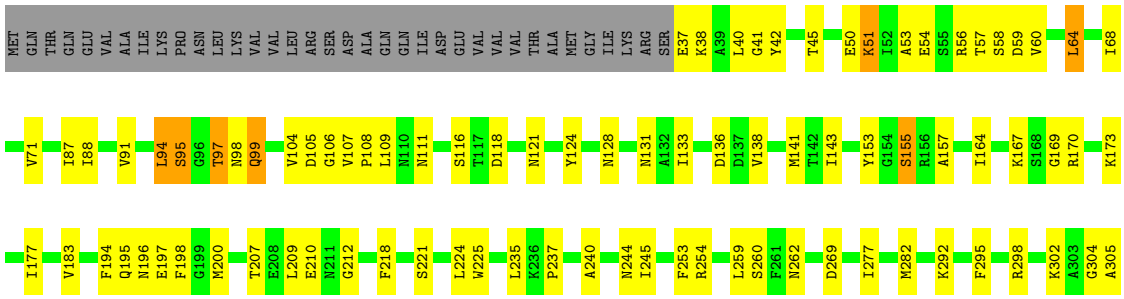
- Molecule 1: PUTATIVE LIPOPROTEIN

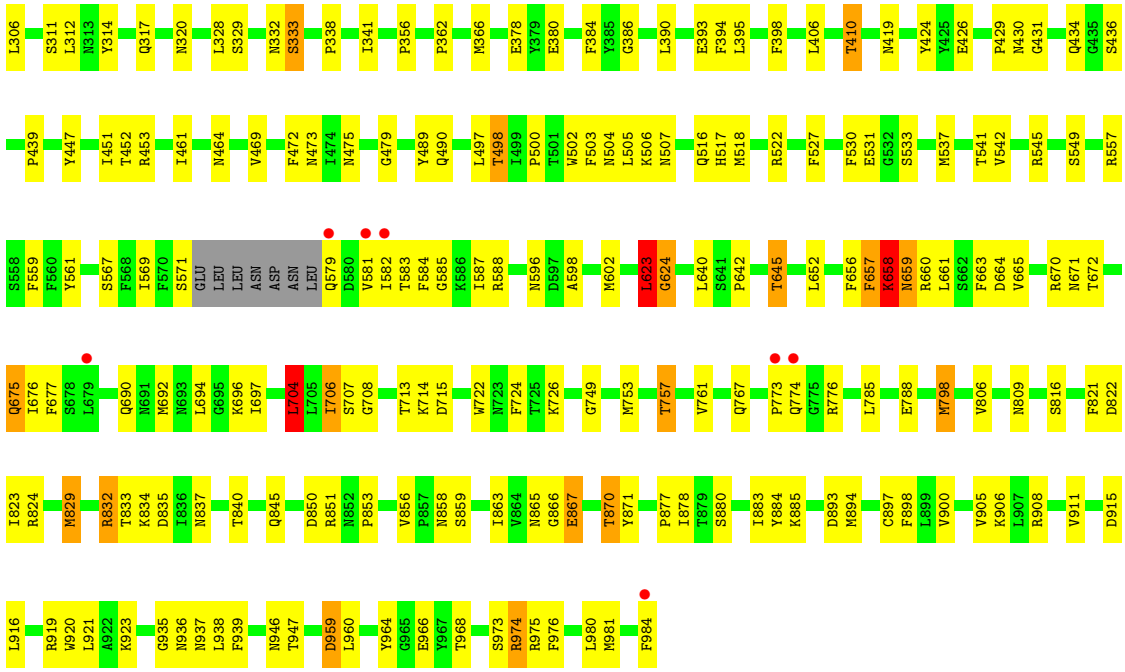
Chain L:



- Molecule 2: SUSC/RAGA FAMILY TONB-LINKED OUTER MEMBRANE PROTEIN

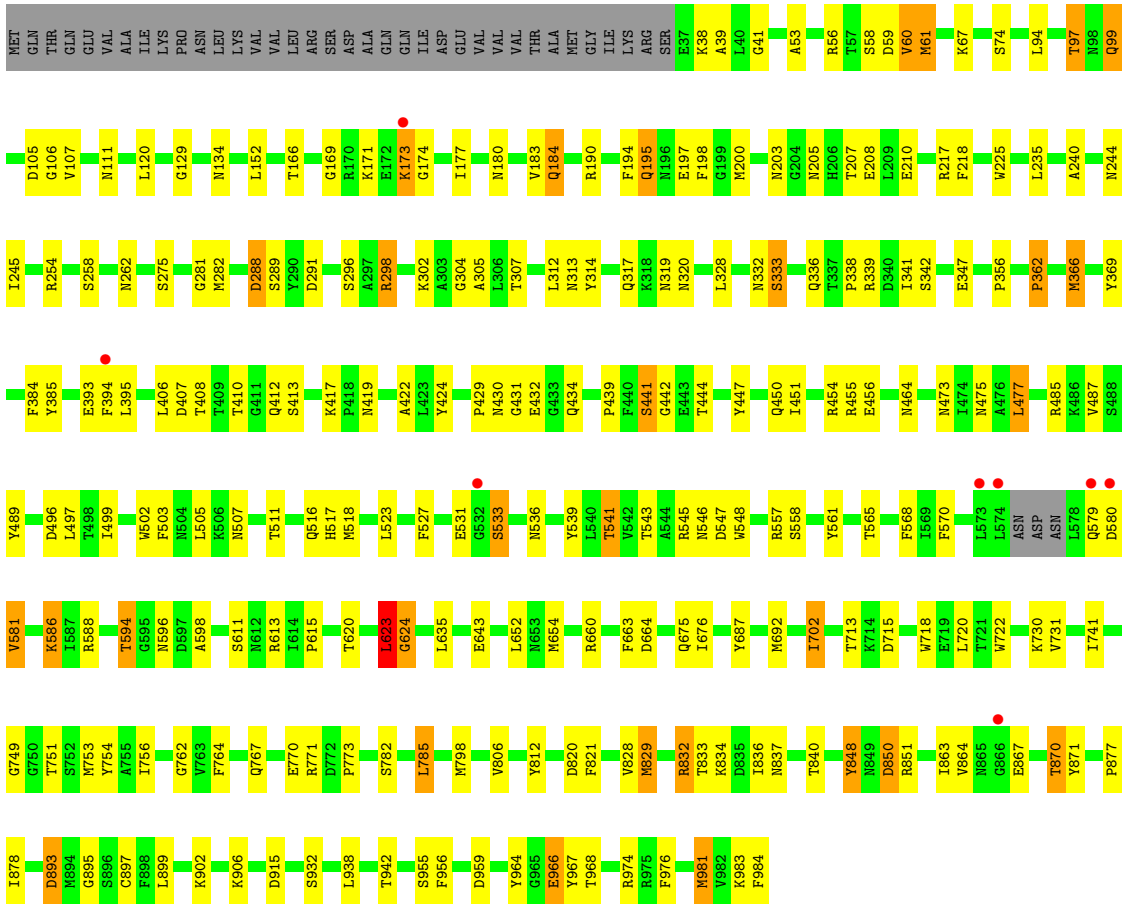
Chain B:





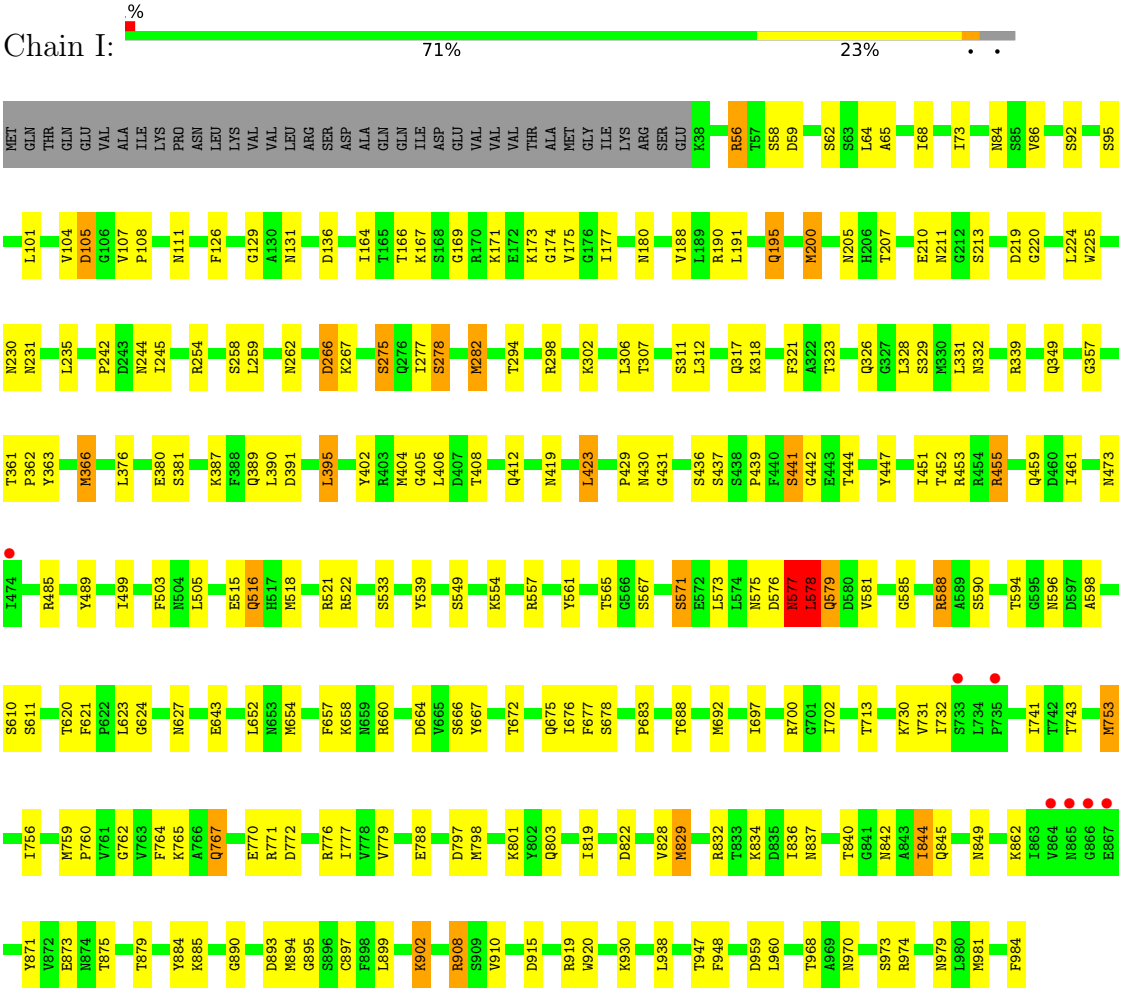
- Molecule 2: SUSC/RAGA FAMILY TONB-LINKED OUTER MEMBRANE PROTEIN

Chain D:



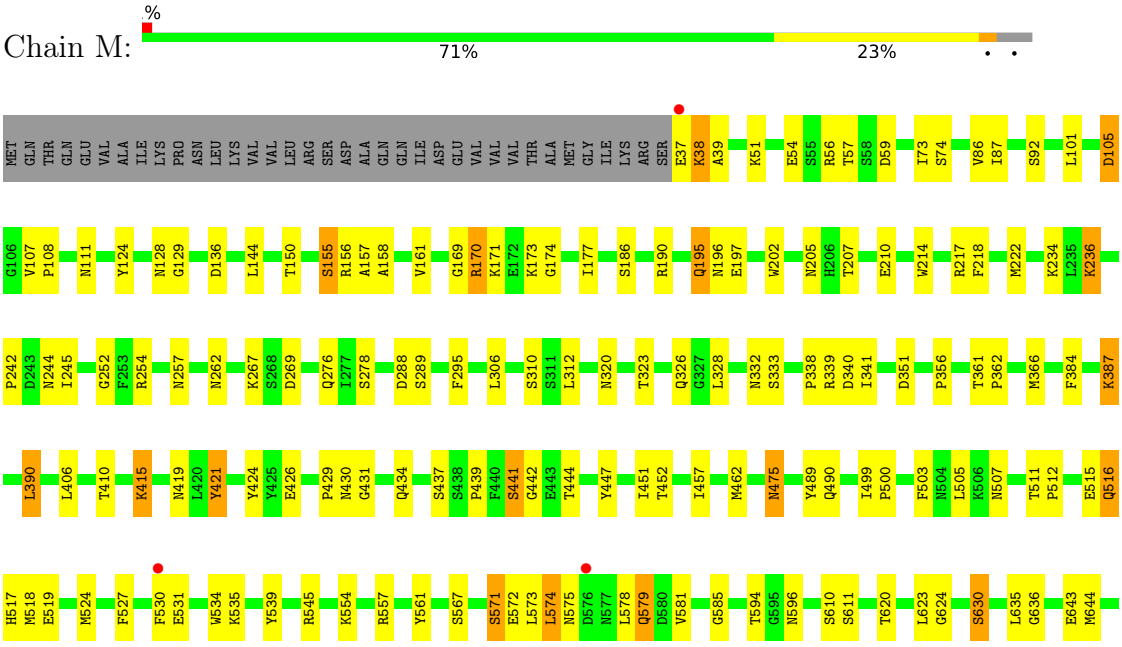
• Molecule 2: SUSC/RAGA FAMILY TONB-LINKED OUTER MEMBRANE PROTEIN

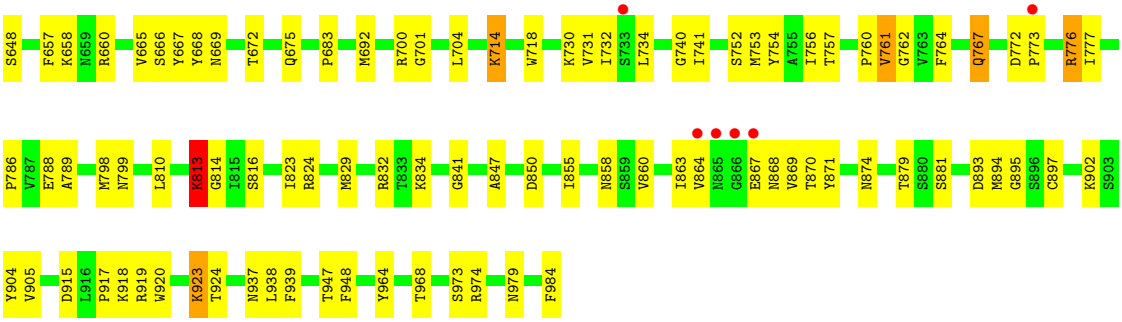
Chain I:



• Molecule 2: SUSC/RAGA FAMILY TONB-LINKED OUTER MEMBRANE PROTEIN

Chain M:



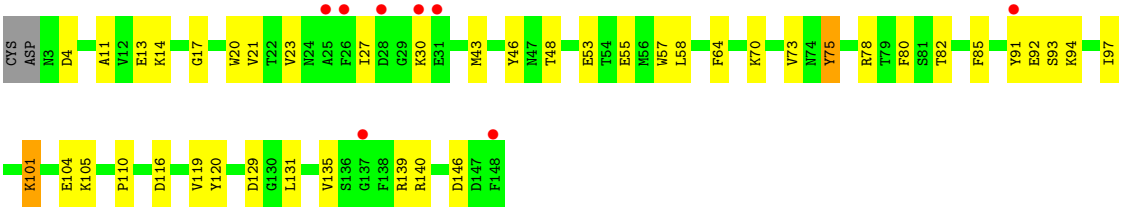


- Molecule 3: UNCHARACTERIZED PROTEIN

Chain E:

- Molecule 3: UNCHARACTERIZED PROTEIN

Chain F:

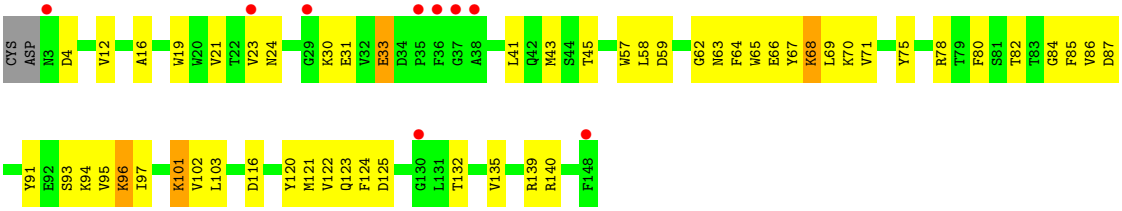


- Molecule 3: UNCHARACTERIZED PROTEIN

Chain J:

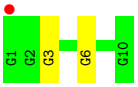
- Molecule 3: UNCHARACTERIZED PROTEIN

Chain N:



• Molecule 4: BT_2261

Chain G:



• Molecule 4: BT_2261

Chain K:

• Molecule 4: BT_2261

Chain O:

• Molecule 4: BT_2261

Chain P:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	222.03Å 91.94Å 261.22Å 90.00° 98.23° 90.00°	Depositor
Resolution (Å)	48.80 – 2.80 48.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.80-2.80) 91.5 (48.80-2.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.198 , 0.255 0.200 , 0.257	Depositor DCC
R_{free} test set	10274 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	1.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49282	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.10 % 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 5.8863e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, NA, KR0

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	0/3843	0.56	0/5231
1	C	0.41	0/3843	0.59	0/5231
1	H	0.42	0/3843	0.59	0/5231
1	L	0.43	0/3843	0.59	0/5231
2	B	0.44	0/7503	0.65	6/10176 (0.1%)
2	D	0.45	1/7536 (0.0%)	0.68	3/10221 (0.0%)
2	I	0.45	0/7552	0.68	4/10245 (0.0%)
2	M	0.46	0/7561	0.67	4/10257 (0.0%)
3	E	0.42	0/1170	0.62	0/1589
3	F	0.40	0/1170	0.59	0/1589
3	J	0.38	0/1170	0.60	0/1589
3	N	0.39	0/1170	0.60	0/1589
4	G	0.55	0/39	1.23	0/47
4	K	0.53	0/39	0.77	0/47
4	O	0.52	0/39	0.86	0/47
4	P	0.57	0/39	0.70	0/47
All	All	0.44	1/50360 (0.0%)	0.64	17/68367 (0.0%)

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
1	H	0	1
1	L	0	2
2	B	0	2
2	D	0	1
2	I	0	2
2	M	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	850	ASP	CB-CG	5.11	1.62	1.51

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	624	GLY	N-CA-C	-8.59	91.64	113.10
2	I	624	GLY	N-CA-C	-7.58	94.16	113.10
2	D	850	ASP	CB-CG-OD1	7.13	124.72	118.30
2	I	578	LEU	CA-CB-CG	7.11	131.66	115.30
2	B	64	LEU	CB-CG-CD1	-6.70	99.61	111.00

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	37	GLU	Peptide
2	B	623	LEU	Peptide
1	C	336	PHE	Peptide
2	D	623	LEU	Peptide
1	H	336	PHE	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	3749	0	3566	90	0
1	C	3749	0	3566	72	0
1	H	3749	0	3566	106	0
1	L	3749	0	3566	146	0
2	B	7326	0	6994	196	0
2	D	7359	0	7033	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	7374	0	7044	160	0
2	M	7383	0	7050	160	0
3	E	1142	0	1056	17	0
3	F	1142	0	1056	27	0
3	J	1142	0	1056	25	0
3	N	1142	0	1056	57	0
4	G	40	0	32	1	0
4	K	40	0	32	3	0
4	O	40	0	32	2	0
4	P	40	0	32	0	0
5	B	27	0	0	0	0
5	D	27	0	0	0	0
5	I	27	0	0	0	0
5	M	27	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	M	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	I	1	0	0	0	0
7	M	1	0	0	0	0
All	All	49282	0	46737	1162	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 12.

The worst 5 of 1162 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:H:211:VAL:HG21	1:H:332:VAL:HG21	1.51	0.92
3:N:85:PHE:HA	3:N:96:LYS:HE3	1.50	0.92
3:N:68:LYS:NZ	3:N:69:LEU:O	2.03	0.91
2:B:302:LYS:NZ	2:B:304:GLY:O	2.04	0.90
3:N:19:TRP:HE1	3:N:45:THR:HG22	1.35	0.89

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	479/480 (100%)	453 (95%)	24 (5%)	2 (0%)	34	66
1	C	479/480 (100%)	452 (94%)	24 (5%)	3 (1%)	25	56
1	H	479/480 (100%)	441 (92%)	35 (7%)	3 (1%)	25	56
1	L	479/480 (100%)	436 (91%)	41 (9%)	2 (0%)	34	66
2	B	937/984 (95%)	880 (94%)	49 (5%)	8 (1%)	17	46
2	D	941/984 (96%)	885 (94%)	54 (6%)	2 (0%)	47	78
2	I	945/984 (96%)	882 (93%)	58 (6%)	5 (0%)	29	61
2	M	946/984 (96%)	893 (94%)	52 (6%)	1 (0%)	51	81
3	E	144/148 (97%)	138 (96%)	6 (4%)	0	100	100
3	F	144/148 (97%)	135 (94%)	9 (6%)	0	100	100
3	J	144/148 (97%)	136 (94%)	6 (4%)	2 (1%)	11	34
3	N	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	22	53
4	G	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	1
4	K	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
4	O	8/10 (80%)	6 (75%)	0	2 (25%)	0	0
4	P	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	6293/6488 (97%)	5895 (94%)	366 (6%)	32 (0%)	29	61

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	38	LYS
2	B	659	ASN
2	B	866	GLY
2	B	920	TRP
1	C	371	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	393/392 (100%)	370 (94%)	23 (6%)	19	49
1	C	393/392 (100%)	377 (96%)	16 (4%)	30	64
1	H	393/392 (100%)	367 (93%)	26 (7%)	16	44
1	L	393/392 (100%)	356 (91%)	37 (9%)	8	26
2	B	793/836 (95%)	743 (94%)	50 (6%)	18	46
2	D	797/836 (95%)	738 (93%)	59 (7%)	13	37
2	I	799/836 (96%)	753 (94%)	46 (6%)	20	50
2	M	800/836 (96%)	754 (94%)	46 (6%)	20	50
3	E	122/124 (98%)	116 (95%)	6 (5%)	25	57
3	F	122/124 (98%)	117 (96%)	5 (4%)	30	64
3	J	122/124 (98%)	112 (92%)	10 (8%)	11	33
3	N	122/124 (98%)	114 (93%)	8 (7%)	16	44
All	All	5249/5408 (97%)	4917 (94%)	332 (6%)	18	46

5 of 332 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	4	ASP
2	M	310	SER
3	J	96	LYS
1	L	291	GLN
2	M	530	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	131	ASN
2	M	110	ASN
2	I	609	GLN
1	L	56	ASN

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Mol	Chain	Res	Type
2	I	459	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
5	KR0	M	1985	-	26,26,26	1.24	2 (7%)	27,27,27	1.36	4 (14%)
5	KR0	I	1985	-	26,26,26	1.28	2 (7%)	27,27,27	1.32	4 (14%)
5	KR0	D	1985	-	26,26,26	1.25	2 (7%)	27,27,27	1.31	4 (14%)
5	KR0	B	1985	-	26,26,26	1.37	2 (7%)	27,27,27	1.14	3 (11%)

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
5	KR0	M	1985	-	-	8/26/26/26	-
5	KR0	I	1985	-	-	9/26/26/26	-
5	KR0	D	1985	-	-	10/26/26/26	-
5	KR0	B	1985	-	-	6/26/26/26	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1985	KR0	O4-C5	4.89	1.47	1.33
5	B	1985	KR0	O1-C7	4.58	1.46	1.33
5	I	1985	KR0	O1-C7	4.52	1.46	1.33
5	M	1985	KR0	O1-C7	4.41	1.46	1.33
5	D	1985	KR0	O1-C7	4.34	1.46	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	1985	KR0	O1-C7-C12	3.99	124.42	111.91
5	M	1985	KR0	O1-C7-C12	3.60	123.22	111.91
5	D	1985	KR0	O4-C5-C10	3.55	123.06	111.91
5	M	1985	KR0	O4-C5-C10	3.53	122.98	111.91
5	B	1985	KR0	O1-C7-C12	3.27	122.18	111.91

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1985	KR0	O9-C7-O1-C1
5	B	1985	KR0	C12-C7-O1-C1
5	D	1985	KR0	O9-C7-O1-C1
5	D	1985	KR0	C12-C7-O1-C1
5	I	1985	KR0	O9-C7-O1-C1

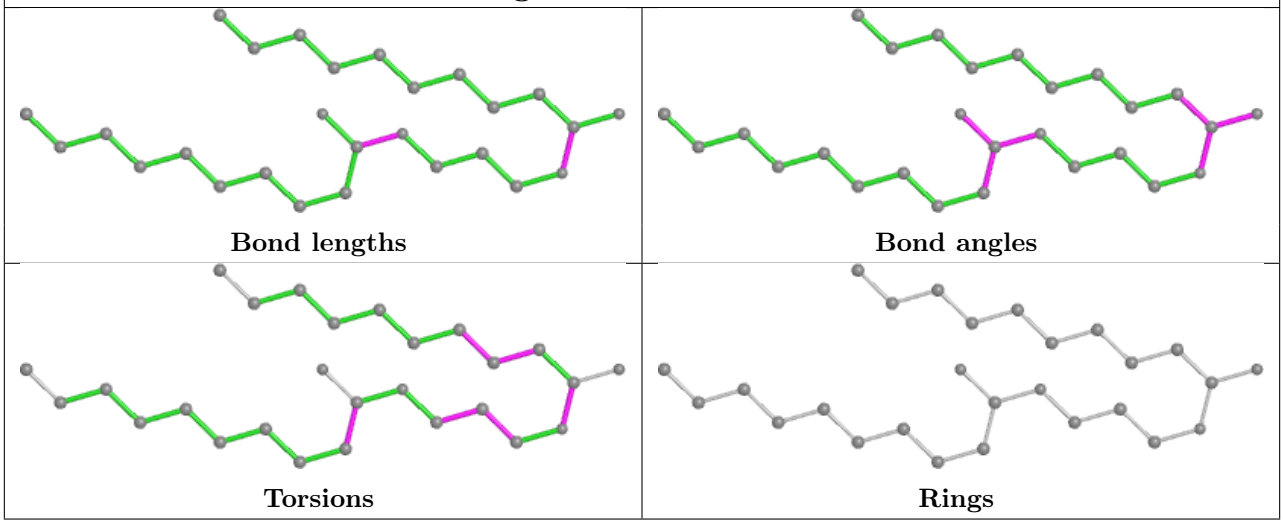
There are no ring outliers.

No monomer is involved in short contacts.

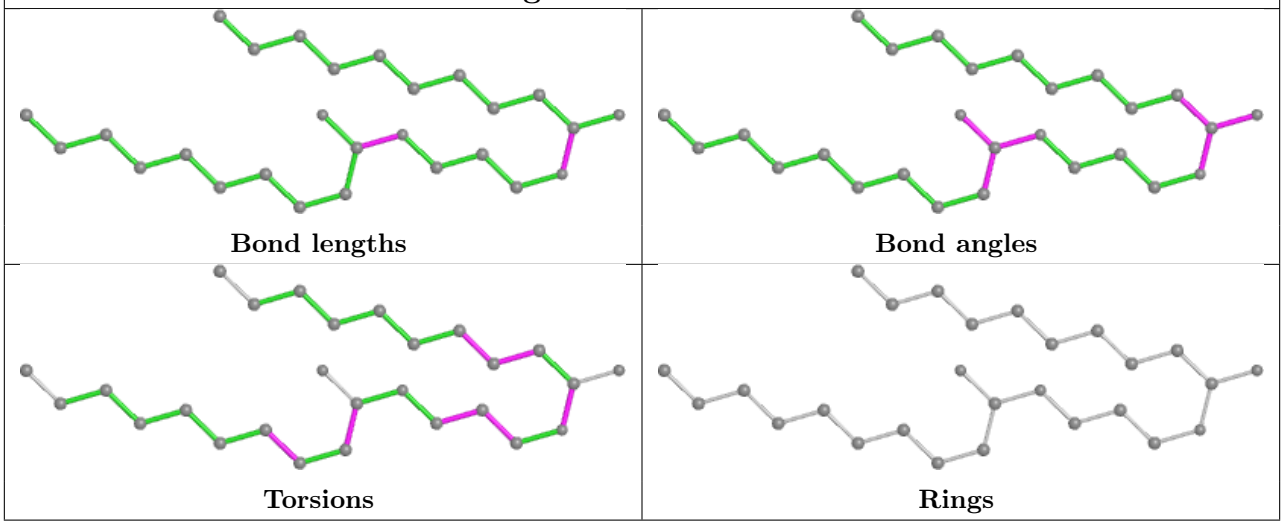
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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

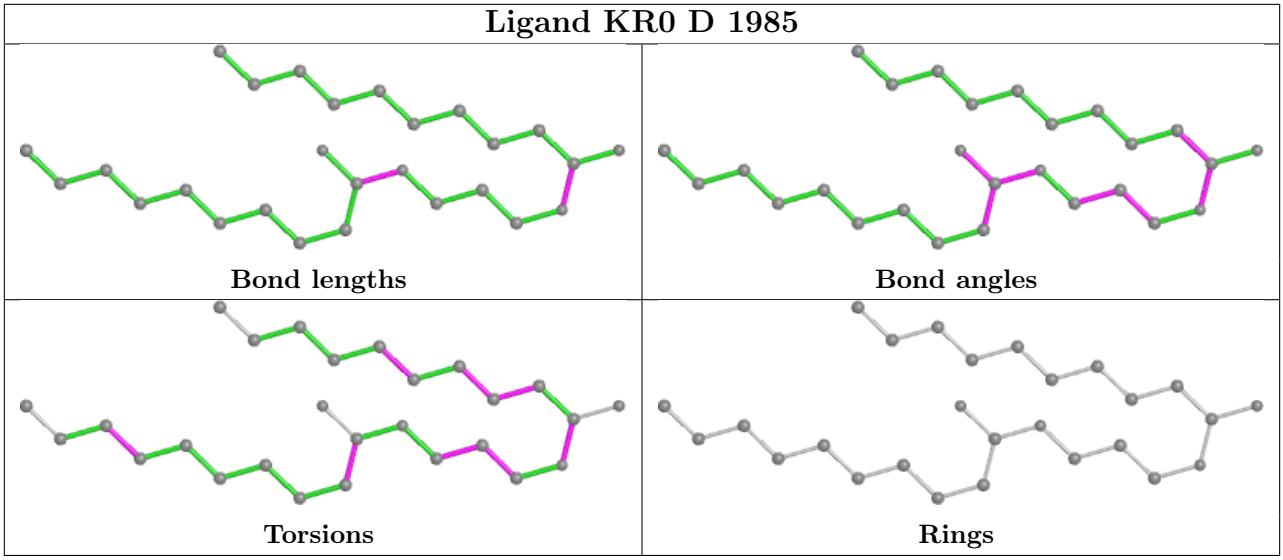
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

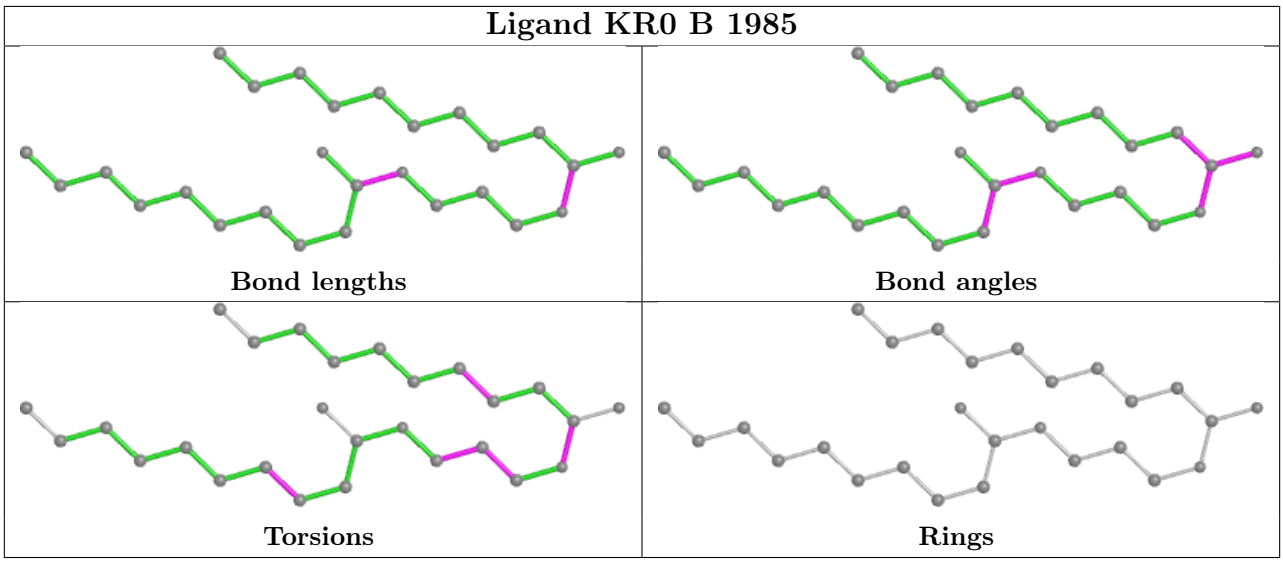
Ligand KR0 M 1985



Ligand KR0 I 1985







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	480/480 (100%)	-0.24	2 (0%)	92	91	43, 66, 98, 161	0
1	C	480/480 (100%)	-0.32	1 (0%)	95	94	35, 57, 87, 116	0
1	H	480/480 (100%)	-0.09	6 (1%)	77	72	39, 68, 101, 166	0
1	L	480/480 (100%)	-0.02	7 (1%)	73	68	40, 77, 115, 171	0
2	B	941/984 (95%)	-0.21	7 (0%)	87	84	35, 60, 96, 135	0
2	D	945/984 (96%)	-0.29	8 (0%)	86	81	31, 50, 80, 154	0
2	I	947/984 (96%)	-0.28	7 (0%)	87	84	32, 52, 81, 160	0
2	M	948/984 (96%)	-0.30	9 (0%)	84	80	31, 51, 79, 172	0
3	E	146/148 (98%)	0.05	1 (0%)	87	84	47, 63, 90, 118	0
3	F	146/148 (98%)	0.36	8 (5%)	25	16	58, 75, 100, 117	0
3	J	146/148 (98%)	0.11	3 (2%)	63	54	56, 81, 108, 154	0
3	N	146/148 (98%)	0.33	9 (6%)	20	13	63, 86, 112, 137	0
4	G	10/10 (100%)	1.37	1 (10%)	7	4	37, 49, 63, 75	0
4	K	10/10 (100%)	1.47	0	100	100	39, 46, 64, 87	0
4	O	10/10 (100%)	1.13	1 (10%)	7	4	38, 51, 73, 88	0
4	P	10/10 (100%)	1.32	0	100	100	41, 50, 62, 96	0
All	All	6325/6488 (97%)	-0.18	70 (1%)	80	75	31, 59, 97, 172	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	866	GLY	11.6
2	M	866	GLY	8.8
1	A	372	CYS	7.2
1	L	372	CYS	7.1
1	H	372	CYS	6.5

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)

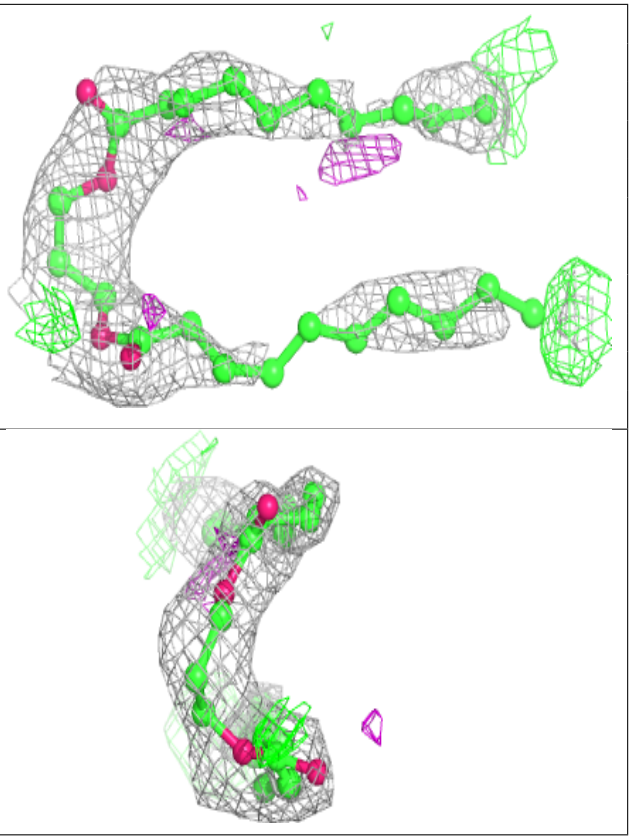
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

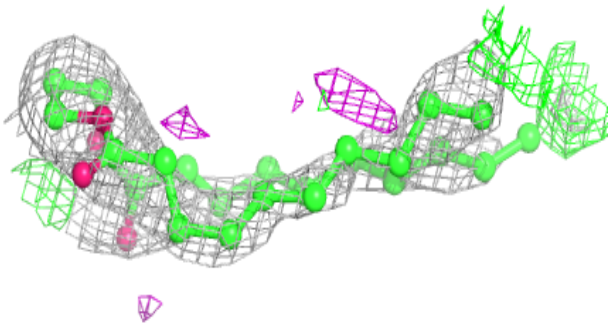
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	KR0	B	1985	27/27	0.82	0.41	52,73,83,89	0
5	KR0	D	1985	27/27	0.84	0.43	46,69,76,78	0
5	KR0	I	1985	27/27	0.85	0.36	43,54,77,87	0
5	KR0	M	1985	27/27	0.86	0.42	42,59,75,81	0
6	NA	M	1986	1/1	0.88	0.29	42,42,42,42	0
7	CA	I	1987	1/1	0.92	0.12	58,58,58,58	0
6	NA	I	1986	1/1	0.93	0.24	32,32,32,32	0
7	CA	M	1987	1/1	0.95	0.31	114,114,114,114	0
6	NA	B	1986	1/1	0.96	0.20	30,30,30,30	0
7	CA	D	1987	1/1	0.97	0.10	47,47,47,47	0
7	CA	B	1987	1/1	0.98	0.10	51,51,51,51	0
6	NA	D	1986	1/1	0.98	0.20	34,34,34,34	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 KR0 B 1985:

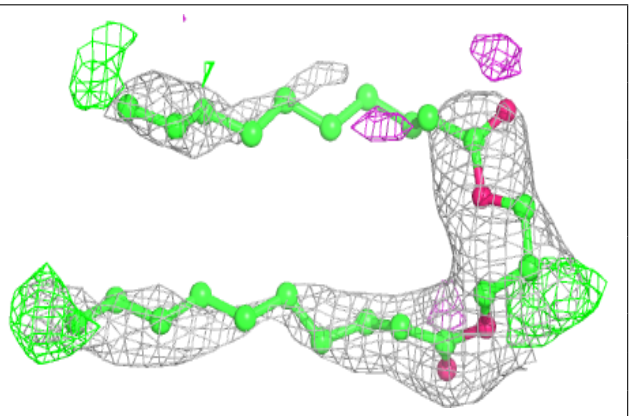
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

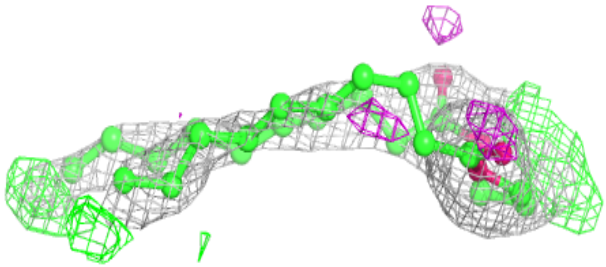


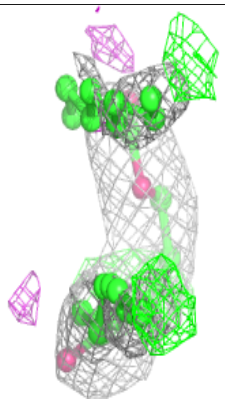


Electron density around KR0 D 1985:

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







Electron density around KR0 I 1985:

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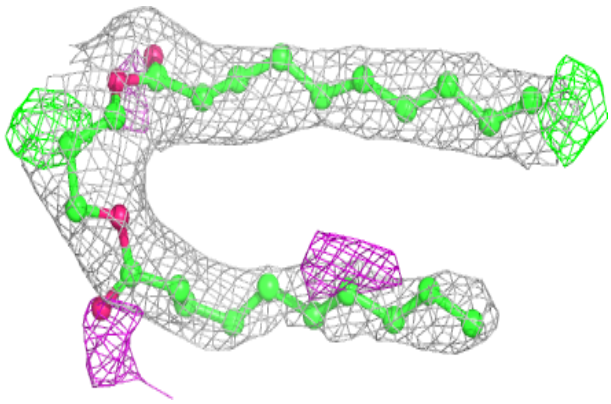
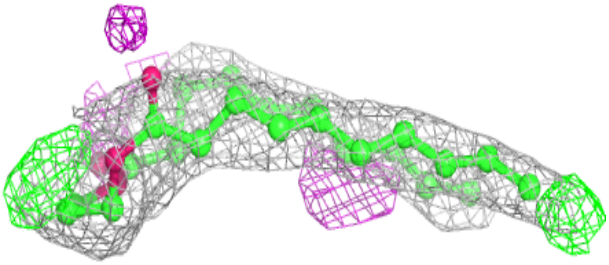
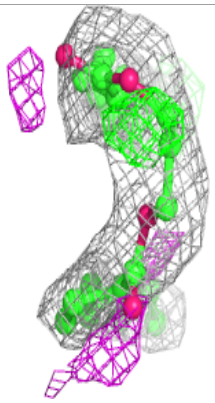
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

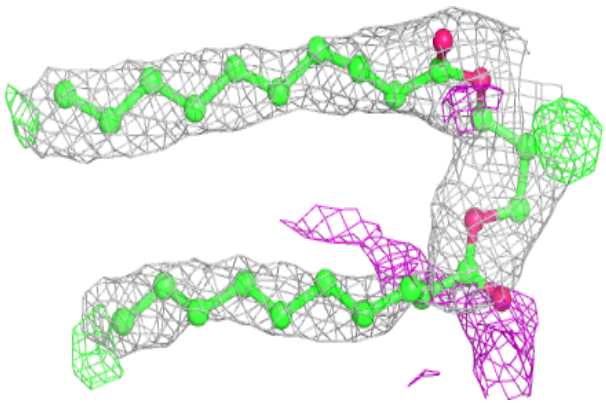


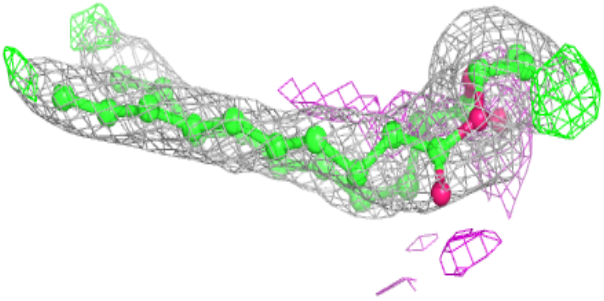


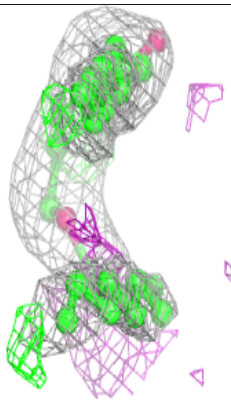


Electron density around KR0 M 1985:

$2mF_o$-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.