



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:22 AM UTC

PDB ID : 2CFH / pdb_00002cfh
Title : Structure of the Bet3-TPC6B core of TRAPP
Authors : Kummel, D.; Muller, J.J.; Roske, Y.; Henke, N.; Heinemann, U.
Deposited on : 2006-02-21
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

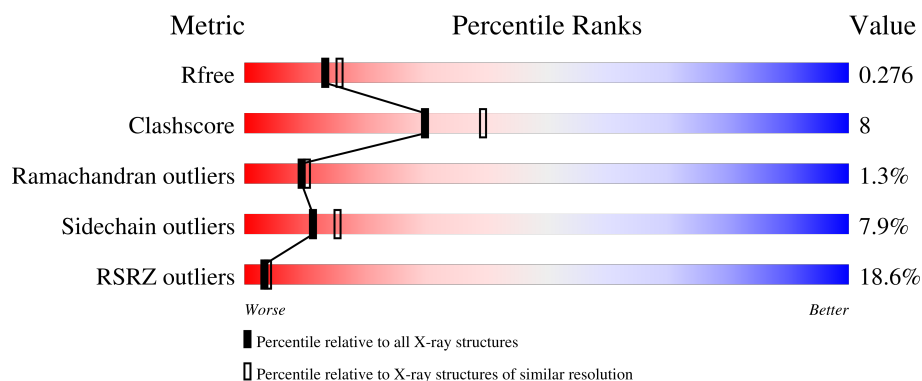
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 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	194	12% 66% 14% • 16%
1	B	194	17% 69% 13% • 16%
2	C	158	20% 70% 20% 5% •
2	D	158	18% 67% 23% • • •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5049 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.

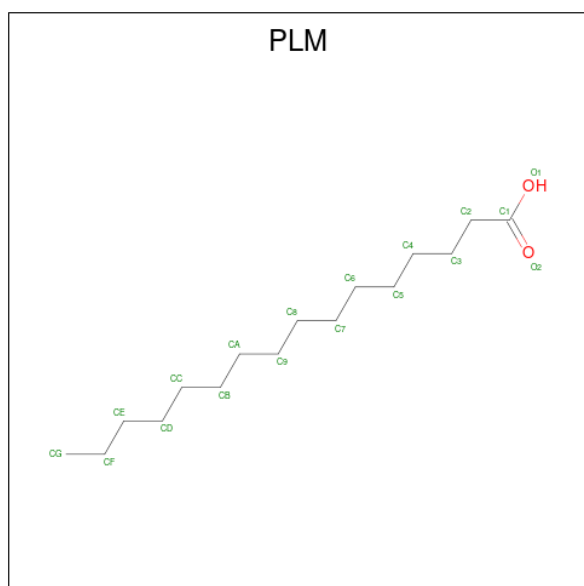
- Molecule 1 is a protein called TRAFFICKING PROTEIN PARTICLE COMPLEX SUB-UNIT 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	1
			1276	807	215	246	8			
1	B	162	Total	C	N	O	S	0	0	1
			1276	807	215	246	8			

- Molecule 2 is a protein called TRAFFICKING PROTEIN PARTICLE COMPLEX SUB-UNIT 6B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	151	Total	C	N	O	S	0	0	1
			1199	764	206	220	9			
2	D	152	Total	C	N	O	S	0	0	1
			1207	769	207	221	10			

- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	16	1		
3	B	1	Total	C	O	0	0
			17	16	1		

- Molecule 4 is water.

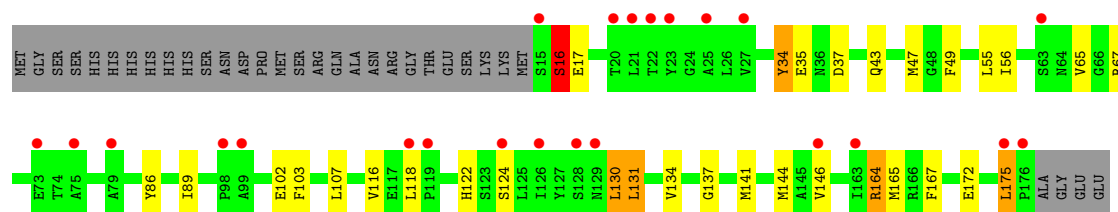
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	12	Total	O	0	0
			12	12		
4	C	10	Total	O	0	0
			10	10		
4	D	17	Total	O	0	0
			17	17		

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.

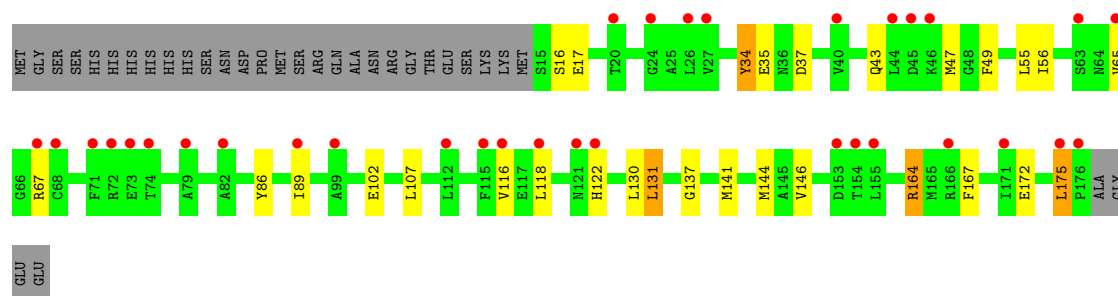
• Molecule 1: TRAFFICKING PROTEIN PARTICLE COMPLEX SUBUNIT 3

Chain A: 



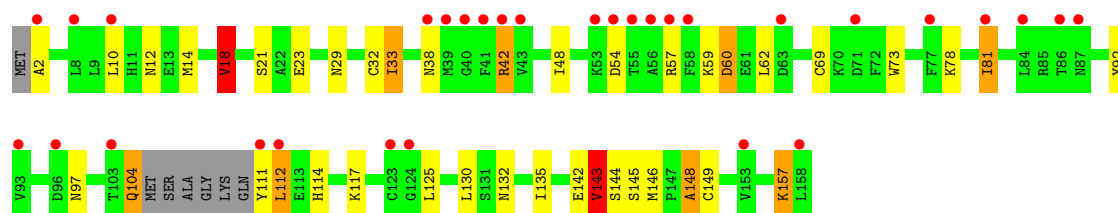
• Molecule 1: TRAFFICKING PROTEIN PARTICLE COMPLEX SUBUNIT 3

Chain B: 



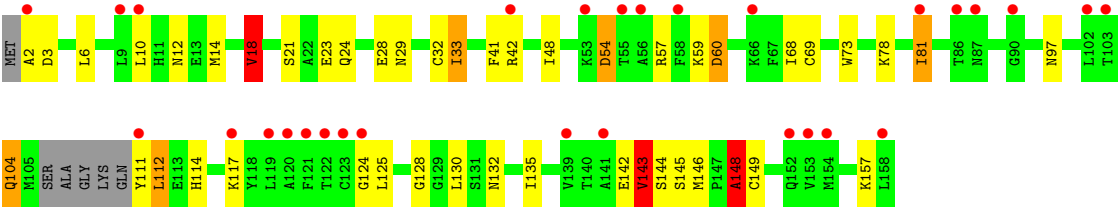
• Molecule 2: TRAFFICKING PROTEIN PARTICLE COMPLEX SUBUNIT 6B

Chain C: 



• Molecule 2: TRAFFICKING PROTEIN PARTICLE COMPLEX SUBUNIT 6B

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.45Å 69.59Å 144.01Å 90.00° 91.55° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.30) 98.6 (20.00-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.269 0.230 , 0.276	Depositor DCC
R_{free} test set	1513 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5049	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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 34.02 % 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 7.2959e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.87	1/1296 (0.1%)	1.02	4/1752 (0.2%)
1	B	0.87	1/1296 (0.1%)	1.02	4/1752 (0.2%)
2	C	1.08	5/1209 (0.4%)	1.08	4/1619 (0.2%)
2	D	0.99	2/1217 (0.2%)	1.04	6/1629 (0.4%)
All	All	0.95	9/5018 (0.2%)	1.04	18/6752 (0.3%)

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	A	0	1
1	B	0	1
2	C	0	1
2	D	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	157	LYS	CE-NZ	17.24	2.01	1.49
2	C	157	LYS	CG-CD	7.78	1.75	1.52
2	D	157	LYS	C-N	-7.08	1.23	1.33
2	C	157	LYS	C-N	-7.03	1.23	1.33
2	C	157	LYS	CD-CE	6.76	1.72	1.52
1	B	175	LEU	C-N	-6.70	1.23	1.34
1	A	175	LEU	C-N	-6.60	1.24	1.34
2	D	143	VAL	CA-CB	6.08	1.60	1.53
2	C	143	VAL	CA-CB	5.57	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	CA-C-N	12.98	139.68	122.42
1	B	67	ARG	C-N-CA	12.98	139.68	122.42
1	A	67	ARG	CA-C-N	12.79	139.43	122.42
1	A	67	ARG	C-N-CA	12.79	139.43	122.42
2	C	157	LYS	CD-CE-NZ	-10.96	76.83	111.90
2	D	68	ILE	CB-CA-C	-7.06	102.61	112.14
2	C	157	LYS	CG-CD-CE	-6.49	96.37	111.30
2	C	18	VAL	CB-CA-C	-5.56	102.17	111.29
2	C	143	VAL	CB-CA-C	5.55	117.57	111.08
2	D	143	VAL	CB-CA-C	5.44	117.10	111.23
2	D	148	ALA	CA-C-N	5.42	131.89	121.54
2	D	148	ALA	C-N-CA	5.42	131.89	121.54
2	D	18	VAL	CB-CA-C	-5.38	102.47	111.29
1	A	17	GLU	N-CA-C	-5.20	105.04	111.33
2	D	54	ASP	N-CA-C	-5.19	104.11	110.65
1	A	34	TYR	N-CA-C	5.08	119.55	112.90
1	B	17	GLU	N-CA-C	-5.06	105.21	111.33
1	B	34	TYR	N-CA-C	5.04	119.45	112.45

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	SER	Peptide
1	B	16	SER	Peptide
2	C	148	ALA	Peptide
2	D	148	ALA	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1276	0	1263	21	0
1	B	1276	0	1263	14	0
2	C	1199	0	1208	32	0
2	D	1207	0	1217	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	17	0	31	1	0
3	B	17	0	31	2	0
4	A	18	0	0	0	0
4	B	12	0	0	0	0
4	C	10	0	0	0	0
4	D	17	0	0	0	0
All	All	5049	0	5013	85	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 8.

All (85) 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)
2:C:157:LYS:CD	2:C:157:LYS:CG	1.75	1.57
2:C:32:CSO:OD	2:C:32:CSO:SG	1.92	1.28
2:D:32:CSO:OD	2:D:32:CSO:SG	1.93	1.25
2:C:157:LYS:NZ	2:C:157:LYS:CE	2.01	1.24
2:C:157:LYS:CD	2:C:157:LYS:NZ	2.33	0.92
2:C:69:CYS:HA	2:C:81:ILE:HD11	1.52	0.91
2:D:69:CYS:HA	2:D:81:ILE:HD11	1.51	0.91
2:C:157:LYS:CG	2:C:157:LYS:CE	2.59	0.80
2:C:157:LYS:CD	2:C:157:LYS:CB	2.60	0.79
2:D:21:SER:OG	2:D:29:ASN:ND2	2.27	0.67
2:D:69:CYS:HA	2:D:81:ILE:CD1	2.25	0.65
2:C:21:SER:OG	2:C:29:ASN:ND2	2.31	0.64
2:C:69:CYS:HA	2:C:81:ILE:CD1	2.28	0.62
1:A:16:SER:HB3	2:C:2:ALA:HB3	1.82	0.61
1:B:34:TYR:O	1:B:35:GLU:HG2	2.01	0.61
1:B:55:LEU:HD11	1:B:86:TYR:CE1	2.39	0.57
1:A:89:ILE:HD12	1:A:107:LEU:HD22	1.88	0.56
1:B:55:LEU:HD11	1:B:86:TYR:CZ	2.42	0.55
1:A:56:ILE:HG21	1:A:141:MET:HB2	1.87	0.54
1:A:55:LEU:HD11	1:A:86:TYR:CE1	2.41	0.54
1:B:56:ILE:HG21	1:B:141:MET:HB2	1.89	0.54
2:C:143:VAL:HG23	2:C:148:ALA:O	2.08	0.54
2:D:97:ASN:HA	2:D:148:ALA:HB2	1.90	0.53
1:A:47:MET:HE3	2:C:18:VAL:CG2	2.39	0.53
1:B:86:TYR:HA	2:D:3:ASP:HB2	1.91	0.51
1:A:16:SER:HB2	2:C:2:ALA:O	2.09	0.51
2:D:69:CYS:SG	2:D:81:ILE:HG13	2.50	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:97:ASN:HA	2:C:148:ALA:HB2	1.92	0.51
1:B:43:GLN:HE21	1:B:47:MET:HG3	1.77	0.50
1:A:34:TYR:O	1:A:35:GLU:HG2	2.12	0.50
1:B:89:ILE:HD12	1:B:107:LEU:HD22	1.93	0.50
1:A:102:GLU:OE1	1:A:164:ARG:NH1	2.45	0.50
2:C:130:LEU:HB3	2:C:135:ILE:HB	1.93	0.50
1:B:37:ASP:OD2	1:B:122:HIS:HA	2.12	0.49
1:A:55:LEU:HD11	1:A:86:TYR:CZ	2.49	0.47
2:C:60:ASP:OD1	2:C:60:ASP:C	2.56	0.47
1:B:49:PHE:CE1	1:B:137:GLY:HA2	2.48	0.47
1:A:49:PHE:CE1	1:A:137:GLY:HA2	2.50	0.47
1:A:47:MET:HE3	2:C:18:VAL:HG22	1.96	0.47
1:B:144:MET:HE2	1:B:167:PHE:CE1	2.50	0.47
2:C:73:TRP:CG	2:C:81:ILE:HD13	2.49	0.47
1:B:102:GLU:OE1	1:B:164:ARG:NH1	2.48	0.46
2:C:62:LEU:HD22	2:C:92:TYR:OH	2.15	0.46
2:D:143:VAL:HG23	2:D:148:ALA:O	2.15	0.46
2:C:69:CYS:SG	2:C:81:ILE:HG13	2.56	0.46
2:D:14:MET:HA	2:D:18:VAL:HG23	1.98	0.46
2:D:111:TYR:CD2	2:D:112:LEU:N	2.84	0.46
2:D:130:LEU:HB3	2:D:135:ILE:HB	1.97	0.46
2:D:73:TRP:CG	2:D:81:ILE:HD13	2.52	0.45
1:A:37:ASP:OD2	1:A:122:HIS:HA	2.16	0.45
2:C:111:TYR:CD2	2:C:112:LEU:N	2.85	0.45
2:D:48:ILE:HG21	2:D:132:ASN:HB3	1.99	0.45
2:C:48:ILE:HG21	2:C:132:ASN:HB3	1.98	0.44
2:D:24:GLN:HB2	2:D:28:GLU:OE1	2.18	0.44
1:A:47:MET:CE	2:C:18:VAL:CG2	2.95	0.44
2:C:114:HIS:HB3	2:C:117:LYS:HD2	1.99	0.44
1:A:16:SER:CB	2:C:2:ALA:HB3	2.48	0.44
2:C:38:ASN:O	2:C:42:ARG:NE	2.51	0.43
1:A:131:LEU:HD21	3:A:1068:PLM:HC2	1.98	0.43
2:D:12:ASN:HB2	2:D:104:GLN:HG3	2.00	0.43
2:D:145:SER:O	2:D:146:MET:C	2.60	0.43
2:D:60:ASP:OD1	2:D:60:ASP:C	2.62	0.43
2:D:33:ILE:HD13	2:D:33:ILE:HA	1.85	0.43
1:A:103:PHE:CZ	1:A:165:MET:HG3	2.53	0.43
2:C:59:LYS:O	2:C:60:ASP:HB3	2.19	0.43
2:C:33:ILE:HD13	2:C:33:ILE:HA	1.86	0.43
2:C:145:SER:O	2:C:146:MET:C	2.62	0.42
2:C:12:ASN:HB2	2:C:104:GLN:HG3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:14:MET:HA	2:C:18:VAL:HG23	2.01	0.42
2:D:41:PHE:CE1	2:D:128:GLY:HA2	2.55	0.42
2:C:23:GLU:HA	2:C:29:ASN:HD21	1.85	0.42
2:D:23:GLU:HA	2:D:29:ASN:HD21	1.84	0.41
1:B:86:TYR:O	2:D:2:ALA:HA	2.21	0.41
1:A:130:LEU:O	1:A:134:VAL:HG23	2.20	0.41
1:B:131:LEU:HD21	3:B:1068:PLM:HC2	2.02	0.41
2:D:41:PHE:HA	2:D:124:GLY:O	2.20	0.41
3:B:1068:PLM:HF1	2:D:6:LEU:HD11	2.02	0.41
2:D:59:LYS:O	2:D:60:ASP:HB3	2.21	0.41
1:A:37:ASP:HB2	1:A:124:SER:HB2	2.02	0.41
1:A:43:GLN:NE2	1:A:43:GLN:HA	2.35	0.40
1:A:144:MET:HE2	1:A:167:PHE:CE1	2.55	0.40
1:A:164:ARG:HD3	1:A:164:ARG:HA	1.84	0.40
2:D:114:HIS:HB3	2:D:117:LYS:HD2	2.03	0.40
2:D:21:SER:HG	2:D:29:ASN:HD22	1.66	0.40
1:B:164:ARG:HA	1:B:164:ARG:HD3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	160/194 (82%)	154 (96%)	5 (3%)	1 (1%)	21	27
1	B	160/194 (82%)	154 (96%)	5 (3%)	1 (1%)	21	27
2	C	146/158 (92%)	132 (90%)	11 (8%)	3 (2%)	5	4
2	D	147/158 (93%)	131 (89%)	13 (9%)	3 (2%)	6	5
All	All	613/704 (87%)	571 (93%)	34 (6%)	8 (1%)	9	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	60	ASP
2	C	149	CYS
2	D	60	ASP
2	D	149	CYS
2	C	112	LEU
2	D	112	LEU
1	A	175	LEU
1	B	175	LEU

5.3.2 Protein sidechains ⓘ

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	142/170 (84%)	133 (94%)	9 (6%)	16	23
1	B	142/170 (84%)	134 (94%)	8 (6%)	19	28
2	C	129/136 (95%)	116 (90%)	13 (10%)	7	9
2	D	130/136 (96%)	117 (90%)	13 (10%)	7	9
All	All	543/612 (89%)	500 (92%)	43 (8%)	11	15

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	65	VAL
1	A	116	VAL
1	A	118	LEU
1	A	130	LEU
1	A	131	LEU
1	A	146	VAL
1	A	164	ARG
1	A	172	GLU
1	B	65	VAL
1	B	116	VAL
1	B	118	LEU
1	B	130	LEU
1	B	131	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	146	VAL
1	B	164	ARG
1	B	172	GLU
2	C	10	LEU
2	C	18	VAL
2	C	33	ILE
2	C	42	ARG
2	C	54	ASP
2	C	57	ARG
2	C	78	LYS
2	C	81	ILE
2	C	104	GLN
2	C	125	LEU
2	C	142	GLU
2	C	143	VAL
2	C	144	SER
2	D	10	LEU
2	D	18	VAL
2	D	33	ILE
2	D	42	ARG
2	D	54	ASP
2	D	57	ARG
2	D	78	LYS
2	D	81	ILE
2	D	104	GLN
2	D	125	LEU
2	D	142	GLU
2	D	143	VAL
2	D	144	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
2	C	29	ASN
2	C	38	ASN
2	C	80	GLN
2	D	29	ASN
2	D	38	ASN
2	D	45	GLN
2	D	80	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSO	D	32	2	3,6,7	0.40	0	1,6,8	0.03	0
2	CSO	C	32	2	3,6,7	0.57	0	1,6,8	0.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	D	32	2	-	0/1/5/7	-
2	CSO	C	32	2	-	0/1/5/7	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	32	CSO	1	0
2	C	32	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	PLM	B	1068	1	15,16,17	0.49	0	14,15,17	0.63	0
3	PLM	A	1068	1	15,16,17	0.47	0	14,15,17	0.58	0

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
3	PLM	B	1068	1	-	8/14/14/15	-
3	PLM	A	1068	1	-	8/14/14/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1068	PLM	O2-C1-C2-C3
3	B	1068	PLM	O2-C1-C2-C3
3	B	1068	PLM	CB-CC-CD-CE
3	A	1068	PLM	CB-CC-CD-CE
3	B	1068	PLM	C8-C9-CA-CB
3	A	1068	PLM	CC-CD-CE-CF

Continued on next page...

Continued from previous page...

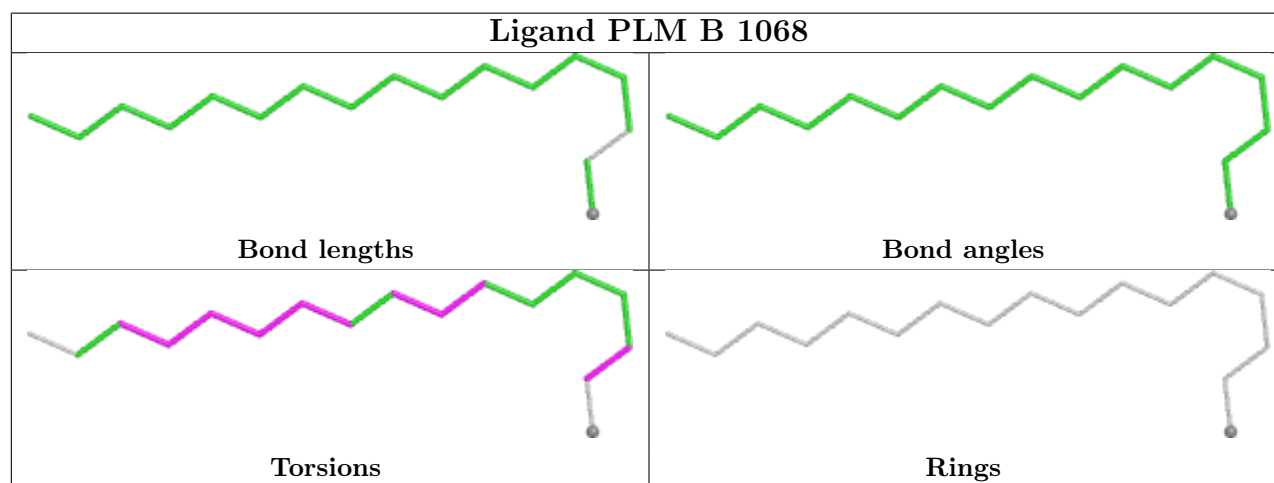
Mol	Chain	Res	Type	Atoms
3	A	1068	PLM	C8-C9-CA-CB
3	B	1068	PLM	CC-CD-CE-CF
3	A	1068	PLM	CA-CB-CC-CD
3	B	1068	PLM	CA-CB-CC-CD
3	B	1068	PLM	C6-C7-C8-C9
3	A	1068	PLM	C6-C7-C8-C9
3	A	1068	PLM	C5-C6-C7-C8
3	B	1068	PLM	C5-C6-C7-C8
3	A	1068	PLM	C9-CA-CB-CC
3	B	1068	PLM	C9-CA-CB-CC

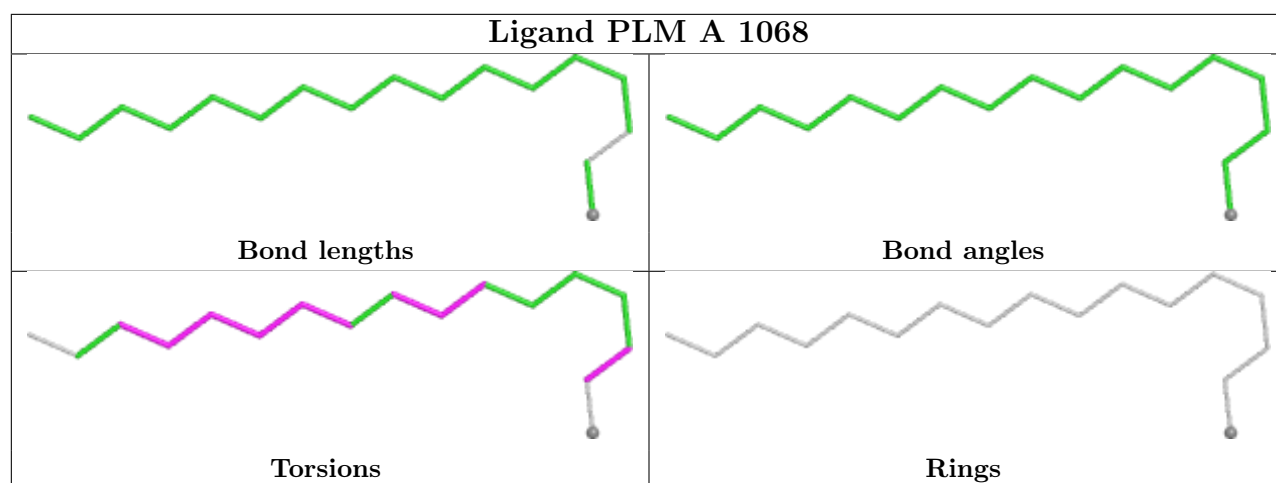
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1068	PLM	2	0
3	A	1068	PLM	1	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 [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	162/194 (83%)	1.16	23 (14%) 6 7	57, 59, 60, 61	0
1	B	162/194 (83%)	1.31	33 (20%) 3 3	57, 59, 61, 62	0
2	C	150/158 (94%)	1.29	31 (20%) 2 3	54, 59, 61, 64	0
2	D	151/158 (95%)	1.45	29 (19%) 3 3	54, 59, 61, 65	0
All	All	625/704 (88%)	1.30	116 (18%) 3 4	54, 59, 61, 65	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	124	GLY	7.5
2	D	121	PHE	6.6
1	A	176	PRO	5.9
2	D	158	LEU	5.8
2	D	123	CYS	5.7
2	D	120	ALA	5.4
2	D	56	ALA	5.2
2	D	153	VAL	4.9
1	A	99	ALA	4.7
2	C	86	THR	4.4
2	C	56	ALA	4.3
2	C	40	GLY	4.2
1	B	176	PRO	4.2
2	C	58	PHE	4.0
1	A	73	GLU	4.0
1	A	98	PRO	3.8
2	C	87	ASN	3.8
2	C	55	THR	3.7
2	D	87	ASN	3.6
2	C	103	THR	3.4
2	D	152	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	122	THR	3.4
2	C	38	ASN	3.4
2	D	58	PHE	3.3
1	B	24	GLY	3.3
1	B	74	THR	3.3
2	D	119	LEU	3.3
2	D	139	VAL	3.3
2	C	41	PHE	3.2
1	B	71	PHE	3.2
2	D	103	THR	3.2
1	B	63	SER	3.1
2	C	2	ALA	3.1
2	D	141	ALA	3.0
1	B	65	VAL	3.0
1	B	68	CYS	3.0
2	C	111	TYR	3.0
2	C	158	LEU	2.9
2	C	42	ARG	2.9
1	A	25	ALA	2.9
2	C	43	VAL	2.9
1	B	73	GLU	2.9
1	A	23	TYR	2.8
1	B	99	ALA	2.8
2	D	66	LYS	2.8
2	C	153	VAL	2.8
2	C	39	MET	2.7
2	C	93	VAL	2.7
2	C	54	ASP	2.7
2	D	86	THR	2.7
2	D	53	LYS	2.6
1	A	22	THR	2.6
1	A	124	SER	2.6
2	C	77	PHE	2.6
2	C	53	LYS	2.6
1	A	27	VAL	2.6
1	B	122	HIS	2.6
1	B	155	LEU	2.6
2	D	42	ARG	2.6
1	B	20	THR	2.6
1	B	116	VAL	2.5
2	C	57	ARG	2.5
1	A	175	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	10	LEU	2.5
2	C	81	ILE	2.5
2	C	84	LEU	2.4
2	D	10	LEU	2.4
2	D	102	LEU	2.4
2	C	112	LEU	2.4
1	B	153	ASP	2.4
1	B	121	ASN	2.3
2	C	63	ASP	2.3
1	A	146	VAL	2.3
1	B	46	LYS	2.3
2	C	124	GLY	2.3
1	B	44	LEU	2.3
1	B	45	ASP	2.3
1	B	82	ALA	2.3
1	B	26	LEU	2.3
2	C	8	LEU	2.3
1	B	72	ARG	2.3
2	C	71	ASP	2.2
2	C	123	CYS	2.2
1	A	119	PRO	2.2
1	B	166	ARG	2.2
2	D	90	GLY	2.2
1	A	20	THR	2.2
1	B	112	LEU	2.2
1	B	175	LEU	2.2
2	D	55	THR	2.2
1	A	15	SER	2.2
1	B	118	LEU	2.2
2	D	9	LEU	2.2
1	A	75	ALA	2.2
1	B	154	THR	2.2
2	D	2	ALA	2.2
2	D	111	TYR	2.2
1	A	126	ILE	2.2
1	A	118	LEU	2.1
1	A	129	ASN	2.1
2	D	117	LYS	2.1
1	B	67	ARG	2.1
1	A	79	ALA	2.1
1	A	128	SER	2.1
1	B	79	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	21	LEU	2.1
2	D	81	ILE	2.1
1	A	163	ILE	2.1
1	B	171	ILE	2.1
2	C	96	ASP	2.1
1	B	115	PHE	2.1
1	A	63	SER	2.0
2	D	154	MET	2.0
1	B	89	ILE	2.0
1	B	27	VAL	2.0
1	B	40	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	CSO	C	32	7/8	0.91	0.11	48,57,57,58	0
2	CSO	D	32	7/8	0.96	0.08	48,57,57,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

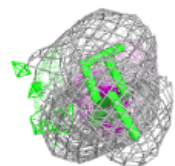
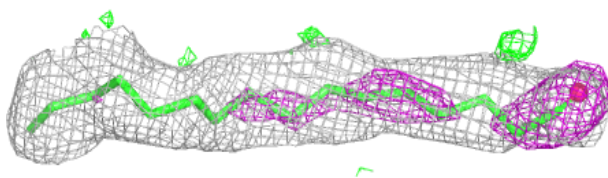
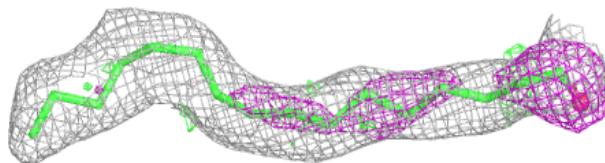
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PLM	A	1068	17/18	0.69	0.16	58,59,61,61	0
3	PLM	B	1068	17/18	0.71	0.17	58,59,61,61	0

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.

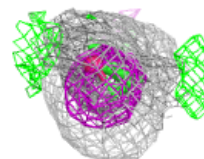
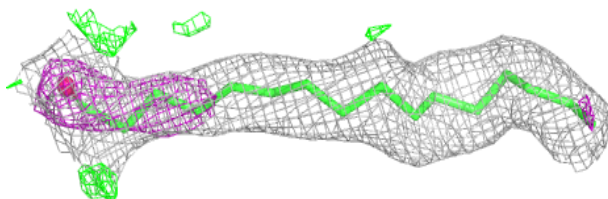
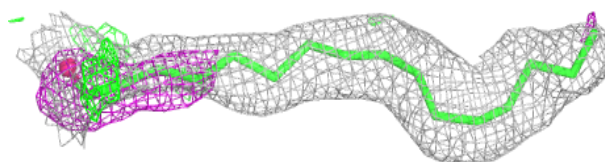
Electron density around PLM A 1068:

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



Electron density around PLM B 1068:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.