



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:13 pm BST

PDB ID : 1GZQ  
Title : CD1b in complex with Phosphatidylinositol  
Authors : Gadola, S.D.; Zaccai, N.R.; Harlos, K.; Shepherd, D.; Ritter, G.; Schmidt, R.R.; Jones, E.Y.; Cerundolo, V.  
Deposited on : 2002-05-24  
Resolution : 2.26 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

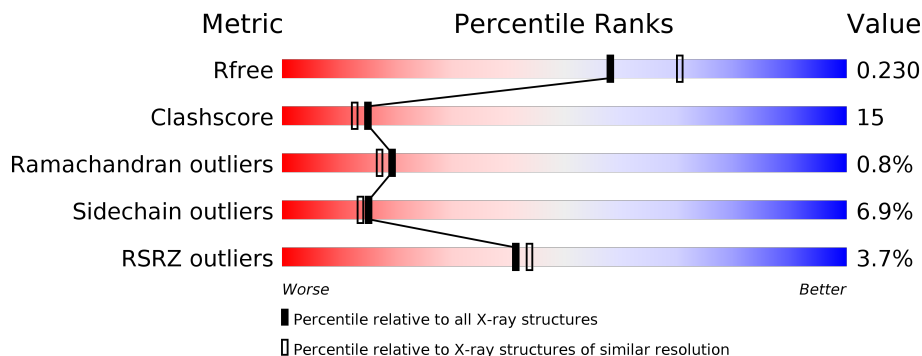
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	300	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">4%      65%      25%      • 7%</p>
2	B	100	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center; margin-top: 5px;">3%      70%      26%      •</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PII	A	1280	-	-	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 3295 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.

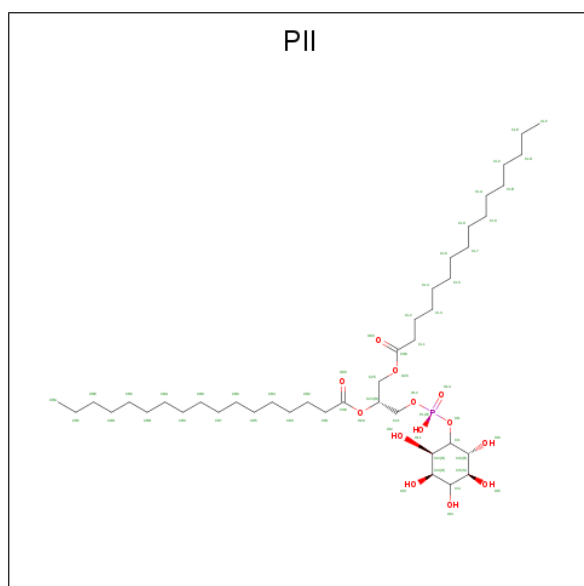
- Molecule 1 is a protein called T-CELL SURFACE GLYCOPROTEIN CD1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	278	2160	1385	366	399	10	0	0	1

- Molecule 2 is a protein called B2-MICROGLOBULIN.

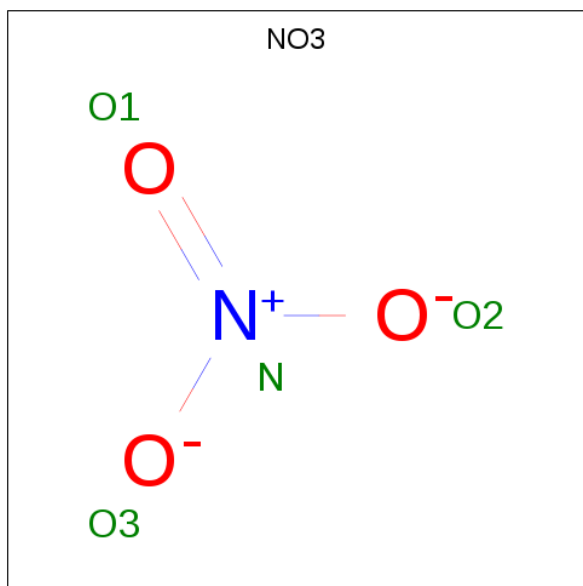
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	0	0	0

- Molecule 3 is 2-[(HYDROXY{[(2R,3R,5S,6R)-2,3,4,5,6-PENTAHYDROXYCYCLOHEXYL]OXY}PHOSPHORYL)OXY]-1-[(PALMITOYLOXY)METHYL]ETHYL HEPTADECANOATE (three-letter code: PII) (formula: C<sub>42</sub>H<sub>81</sub>O<sub>13</sub>P).



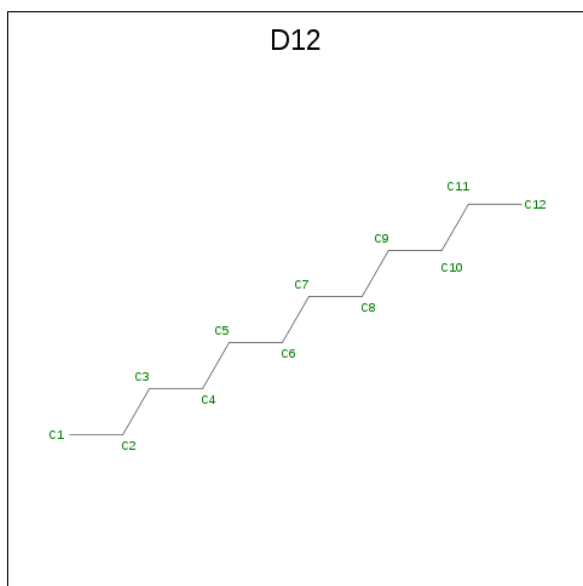
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	56	42	13	1	0	0

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



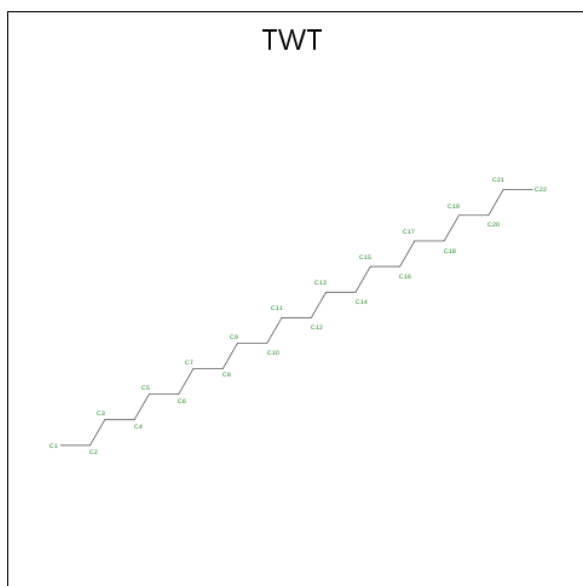
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	A	1	Total	N	O	0	0
			4	1	3		
4	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is DODECANE (three-letter code: D12) (formula: C<sub>12</sub>H<sub>26</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 12 12	0	0

- Molecule 6 is DOCOSANE (three-letter code: TWT) (formula:  $C_{22}H_{46}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 22 22	0	0

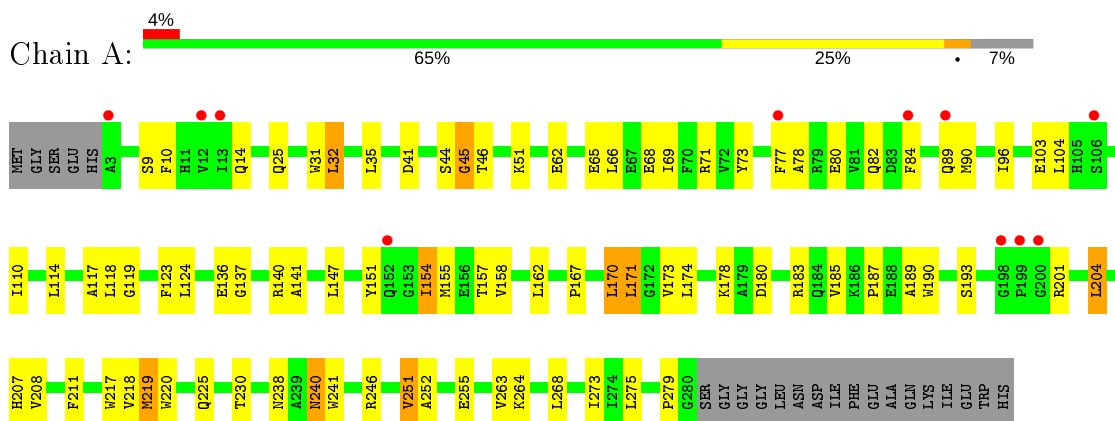
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	139	Total O 139 139	0	0
7	B	57	Total O 57 57	0	0

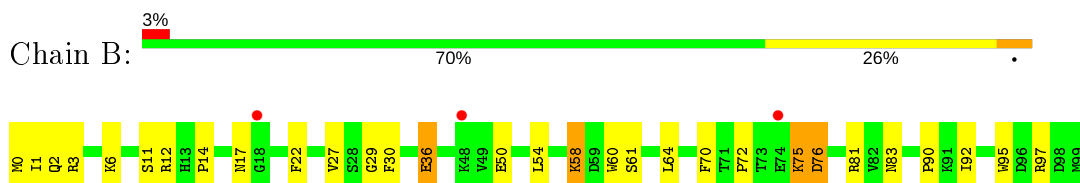
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: T-CELL SURFACE GLYCOPROTEIN CD1B



- Molecule 2: B2-MICROGLOBULIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.88Å 177.00Å 75.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.30 – 2.26 24.30 – 2.21	Depositor EDS
% Data completeness (in resolution range)	91.1 (24.30-2.26) 91.4 (24.30-2.21)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.84 (at 2.22Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.203 , 0.237 0.196 , 0.230	Depositor DCC
$R_{free}$ test set	811 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtrriage
Anisotropy	0.279	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PII, TWT, D12, NO3

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	0.43	0/2221	0.70	1/3017 (0.0%)
2	B	0.42	0/860	0.69	0/1162
All	All	0.42	0/3081	0.70	1/4179 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ASN	N-CA-C	-5.70	95.61	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2160	0	2077	65	0
2	B	837	0	803	22	0
3	A	56	0	80	8	0
4	A	12	0	0	3	0
5	A	12	0	26	6	0
6	A	22	0	46	6	0
7	A	139	0	0	5	0
7	B	57	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3295	0	3032	92	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 15.

All (92) 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:A:1281:NO3:N	4:A:1281:NO3:O3	1.60	1.33
4:A:1283:NO3:O3	4:A:1283:NO3:N	1.61	1.30
4:A:1282:NO3:O3	4:A:1282:NO3:N	1.61	1.28
2:B:58:LYS:H	2:B:58:LYS:HD2	1.14	1.08
1:A:251:VAL:HG22	1:A:255:GLU:HG3	1.50	0.91
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.57	0.87
1:A:80:GLU:HG3	5:A:1284:D12:H31	1.65	0.79
1:A:219:MET:HE2	1:A:230:THR:HG21	1.66	0.77
2:B:58:LYS:CD	2:B:58:LYS:H	1.89	0.75
2:B:83:ASN:OD1	2:B:90:PRO:HG3	1.88	0.74
1:A:240:ASN:HD22	1:A:240:ASN:H	1.37	0.73
1:A:246:ARG:HD3	7:A:2122:HOH:O	1.89	0.71
1:A:183:ARG:NH1	1:A:185:VAL:HG21	2.04	0.71
1:A:44:SER:O	1:A:46:THR:N	2.25	0.70
2:B:58:LYS:N	2:B:58:LYS:HD2	1.98	0.67
1:A:151:TYR:CZ	5:A:1284:D12:H42	2.32	0.64
1:A:90:MET:HE1	5:A:1284:D12:H121	1.79	0.64
1:A:183:ARG:HH11	1:A:185:VAL:CG2	2.13	0.62
1:A:201:ARG:HG2	1:A:201:ARG:HH11	1.66	0.61
2:B:17:ASN:HA	2:B:72:PRO:O	2.01	0.60
3:A:1280:PII:HQ	6:A:1285:TWT:C1	2.32	0.60
1:A:154:ILE:O	1:A:158:VAL:HG23	2.01	0.59
1:A:73:TYR:HE1	3:A:1280:PII:HL51	1.69	0.58
2:B:36:GLU:HG2	2:B:83:ASN:HD22	1.69	0.57
2:B:95:TRP:CH2	2:B:97:ARG:HG2	2.39	0.57
1:A:62:GLU:O	1:A:66:LEU:HD23	2.04	0.57
1:A:183:ARG:HH11	1:A:185:VAL:HG21	1.67	0.57
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.39	0.57
1:A:51:LYS:HE3	1:A:241:TRP:CZ2	2.40	0.57
1:A:155:MET:CE	3:A:1280:PII:HY2	2.35	0.56
1:A:240:ASN:HD22	1:A:240:ASN:N	1.99	0.56
1:A:157:THR:OG1	3:A:1280:PII:HI1	2.07	0.55
1:A:158:VAL:O	1:A:162:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PHE:HZ	1:A:96:ILE:HG21	1.73	0.54
1:A:124:LEU:HD12	1:A:124:LEU:C	2.28	0.54
1:A:78:ALA:O	1:A:82:GLN:HG2	2.09	0.53
1:A:183:ARG:NH1	1:A:185:VAL:CG2	2.71	0.53
1:A:14:GLN:HE21	6:A:1285:TWT:H111	1.74	0.53
2:B:54:LEU:HA	2:B:64:LEU:HD21	1.92	0.52
1:A:217:TRP:HB3	1:A:264:LYS:HB2	1.91	0.51
1:A:201:ARG:HG2	1:A:201:ARG:NH1	2.24	0.51
1:A:123:PHE:CZ	6:A:1285:TWT:H223	2.46	0.51
1:A:180:ASP:O	1:A:183:ARG:HG2	2.11	0.51
1:A:137:GLY:HA3	1:A:141:ALA:HB2	1.91	0.50
1:A:89:GLN:O	1:A:140:ARG:NH2	2.45	0.50
2:B:27:VAL:HG23	2:B:30:PHE:CE1	2.47	0.49
3:A:1280:PII:HQ	6:A:1285:TWT:H1C1	1.95	0.48
1:A:251:VAL:HG22	1:A:255:GLU:CG	2.35	0.48
1:A:157:THR:HG23	3:A:1280:PII:HI3	1.94	0.48
7:A:2119:HOH:O	2:B:12:ARG:HB2	2.14	0.47
1:A:183:ARG:NH2	1:A:241:TRP:HB3	2.28	0.47
1:A:189:ALA:HA	1:A:207:HIS:O	2.14	0.47
1:A:118:LEU:HD13	1:A:119:GLY:N	2.30	0.47
1:A:170:LEU:HD22	1:A:174:LEU:HG	1.96	0.47
1:A:252:ALA:HB3	1:A:255:GLU:HG2	1.96	0.47
2:B:75:LYS:O	2:B:76:ASP:HB2	2.15	0.47
3:A:1280:PII:HQ	6:A:1285:TWT:H1C2	1.97	0.46
2:B:0:MET:HE3	2:B:2:GLN:HG3	1.96	0.46
1:A:45:GLY:HA3	1:A:71:ARG:HD3	1.97	0.46
1:A:154:ILE:C	1:A:154:ILE:HD12	2.37	0.45
1:A:167:PRO:O	1:A:171:LEU:HD22	2.16	0.45
1:A:89:GLN:HB2	7:A:2062:HOH:O	2.16	0.45
1:A:219:MET:HE2	1:A:230:THR:CG2	2.43	0.45
1:A:68:GLU:OE2	1:A:71:ARG:NH1	2.47	0.45
2:B:29:GLY:HA2	2:B:61:SER:OG	2.16	0.45
1:A:114:LEU:HD23	1:A:114:LEU:C	2.37	0.45
1:A:9:SER:O	1:A:32:LEU:HA	2.17	0.44
1:A:118:LEU:C	1:A:118:LEU:HD13	2.38	0.44
1:A:41:ASP:O	1:A:44:SER:O	2.35	0.44
2:B:6:LYS:O	2:B:27:VAL:HA	2.18	0.43
1:A:65:GLU:O	1:A:69:ILE:HG13	2.18	0.43
1:A:25:GLN:NE2	7:A:2020:HOH:O	2.52	0.43
1:A:263:VAL:HB	1:A:273:ILE:HB	2.00	0.43
5:A:1284:D12:C12	6:A:1285:TWT:H221	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HA	1:A:32:LEU:HD12	1.86	0.43
1:A:157:THR:OG1	3:A:1280:PII:HI5	2.18	0.42
2:B:95:TRP:CZ2	2:B:97:ARG:HG2	2.54	0.42
1:A:240:ASN:H	1:A:240:ASN:ND2	2.09	0.42
1:A:208:VAL:HG21	1:A:218:VAL:HG21	2.02	0.42
1:A:204:LEU:HB3	1:A:220:TRP:CZ2	2.55	0.42
1:A:103:GLU:O	1:A:110:ILE:HA	2.20	0.42
1:A:90:MET:CE	5:A:1284:D12:H121	2.48	0.42
1:A:136:GLU:N	1:A:136:GLU:OE1	2.47	0.42
1:A:84:PHE:HB2	5:A:1284:D12:H92	2.01	0.41
2:B:1:ILE:HD12	2:B:3:ARG:HE	1.85	0.41
1:A:190:TRP:CZ3	2:B:14:PRO:HD3	2.55	0.41
1:A:78:ALA:HB2	7:A:2022:HOH:O	2.21	0.41
2:B:81:ARG:HB2	2:B:92:ILE:CD1	2.51	0.41
2:B:11:SER:HA	2:B:22:PHE:O	2.21	0.40
2:B:75:LYS:HA	2:B:75:LYS:HD3	1.74	0.40
2:B:27:VAL:HG23	2:B:30:PHE:HE1	1.86	0.40
1:A:10:PHE:HA	1:A:31:TRP:O	2.21	0.40

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	276/300 (92%)	268 (97%)	6 (2%)	2 (1%)	22	21
2	B	98/100 (98%)	91 (93%)	6 (6%)	1 (1%)	15	13
All	All	374/400 (94%)	359 (96%)	12 (3%)	3 (1%)	19	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLY
2	B	76	ASP
1	A	279	PRO

### 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	226/243 (93%)	209 (92%)	17 (8%)	13	12
2	B	95/95 (100%)	90 (95%)	5 (5%)	22	23
All	All	321/338 (95%)	299 (93%)	22 (7%)	15	14

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	35	LEU
1	A	104	LEU
1	A	147	LEU
1	A	154	ILE
1	A	170	LEU
1	A	171	LEU
1	A	173	VAL
1	A	178	LYS
1	A	193	SER
1	A	204	LEU
1	A	219	MET
1	A	225	GLN
1	A	240	ASN
1	A	251	VAL
1	A	268	LEU
1	A	275	LEU
2	B	36	GLU
2	B	50	GLU
2	B	58	LYS
2	B	70	PHE

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Mol	Chain	Res	Type
2	B	75	LYS

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

Mol	Chain	Res	Type
1	A	14	GLN
1	A	89	GLN
1	A	184	GLN
1	A	225	GLN
1	A	227	GLN
1	A	231	GLN
1	A	240	ASN
2	B	2	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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
5	D12	A	1284	-	11,11,11	0.27	0	10,10,10	0.52	0
4	NO3	A	1283	-	1,3,3	4.82	1 (100%)	0,3,3	0.00	-
4	NO3	A	1282	-	1,3,3	5.26	1 (100%)	0,3,3	0.00	-
4	NO3	A	1281	-	1,3,3	4.89	1 (100%)	0,3,3	0.00	-
6	TWT	A	1285	-	21,21,21	0.26	0	20,20,20	0.56	0
3	PII	A	1280	-	56,56,56	0.98	5 (8%)	66,68,68	0.88	2 (3%)

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	D12	A	1284	-	-	4/9/9/9	-
6	TWT	A	1285	-	-	13/19/19/19	-
3	PII	A	1280	-	-	26/51/75/75	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1282	NO3	O1-N	5.26	1.48	1.24
4	A	1281	NO3	O1-N	4.89	1.46	1.24
4	A	1283	NO3	O1-N	4.82	1.46	1.24
3	A	1280	PII	O29-CO9	-2.77	1.26	1.34
3	A	1280	PII	CI2-CI1	2.43	1.58	1.52
3	A	1280	PII	O26-CO6	-2.31	1.26	1.33
3	A	1280	PII	CI6-CI1	2.25	1.58	1.52
3	A	1280	PII	CI3-CI2	2.22	1.58	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1280	PII	O29-CO9-CR1	3.49	119.01	111.50
3	A	1280	PII	C24-O29-CO9	-3.19	109.93	117.79

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1280	PII	CI2-CI1-OI1-P1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	1280	PII	CI6-CI1-OI1-P1
3	A	1280	PII	C21-O12-P1-O13
3	A	1280	PII	CR1-CO9-O29-C24
3	A	1280	PII	OC6-CO6-O26-C25
3	A	1280	PII	OC9-CO9-O29-C24
3	A	1280	PII	CL1-CO6-O26-C25
3	A	1280	PII	CL2-CL3-CL4-CL5
3	A	1280	PII	CLA-CLB-CLC-CLD
5	A	1284	D12	C2-C3-C4-C5
6	A	1285	TWT	C13-C14-C15-C16
3	A	1280	PII	CL8-CL9-CLA-CLB
6	A	1285	TWT	C14-C15-C16-C17
3	A	1280	PII	CL5-CL6-CL7-CL8
3	A	1280	PII	CL3-CL4-CL5-CL6
3	A	1280	PII	CR1-CR2-CR3-CR4
3	A	1280	PII	CL1-CL2-CL3-CL4
6	A	1285	TWT	C11-C12-C13-C14
6	A	1285	TWT	C9-C10-C11-C12
6	A	1285	TWT	C15-C16-C17-C18
6	A	1285	TWT	C6-C7-C8-C9
5	A	1284	D12	C3-C4-C5-C6
3	A	1280	PII	CR7-CR8-CR9-CRA
3	A	1280	PII	CL9-CLA-CLB-CLC
3	A	1280	PII	CR2-CR3-CR4-CR5
6	A	1285	TWT	C11-C10-C9-C8
3	A	1280	PII	CRD-CRE-CRF-CRG
3	A	1280	PII	CO6-CL1-CL2-CL3
3	A	1280	PII	CRC-CRD-CRE-CRF
6	A	1285	TWT	C5-C6-C7-C8
5	A	1284	D12	C1-C2-C3-C4
5	A	1284	D12	C9-C10-C11-C12
3	A	1280	PII	CRA-CRB-CRC-CRD
6	A	1285	TWT	C18-C19-C20-C21
3	A	1280	PII	CL7-CL8-CL9-CLA
6	A	1285	TWT	C10-C11-C12-C13
3	A	1280	PII	CR9-CRA-CRB-CRC
6	A	1285	TWT	C2-C3-C4-C5
3	A	1280	PII	C21-O12-P1-OI1
3	A	1280	PII	CLC-CLD-CLE-CLF
6	A	1285	TWT	C1-C2-C3-C4
3	A	1280	PII	CR4-CR5-CR6-CR7
6	A	1285	TWT	C16-C17-C18-C19

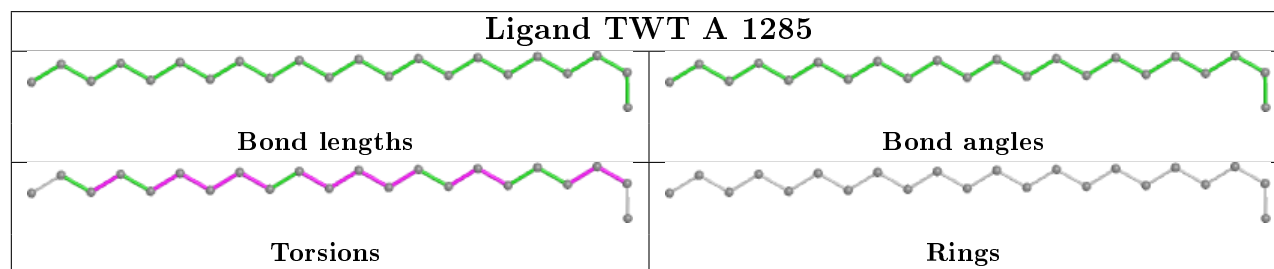


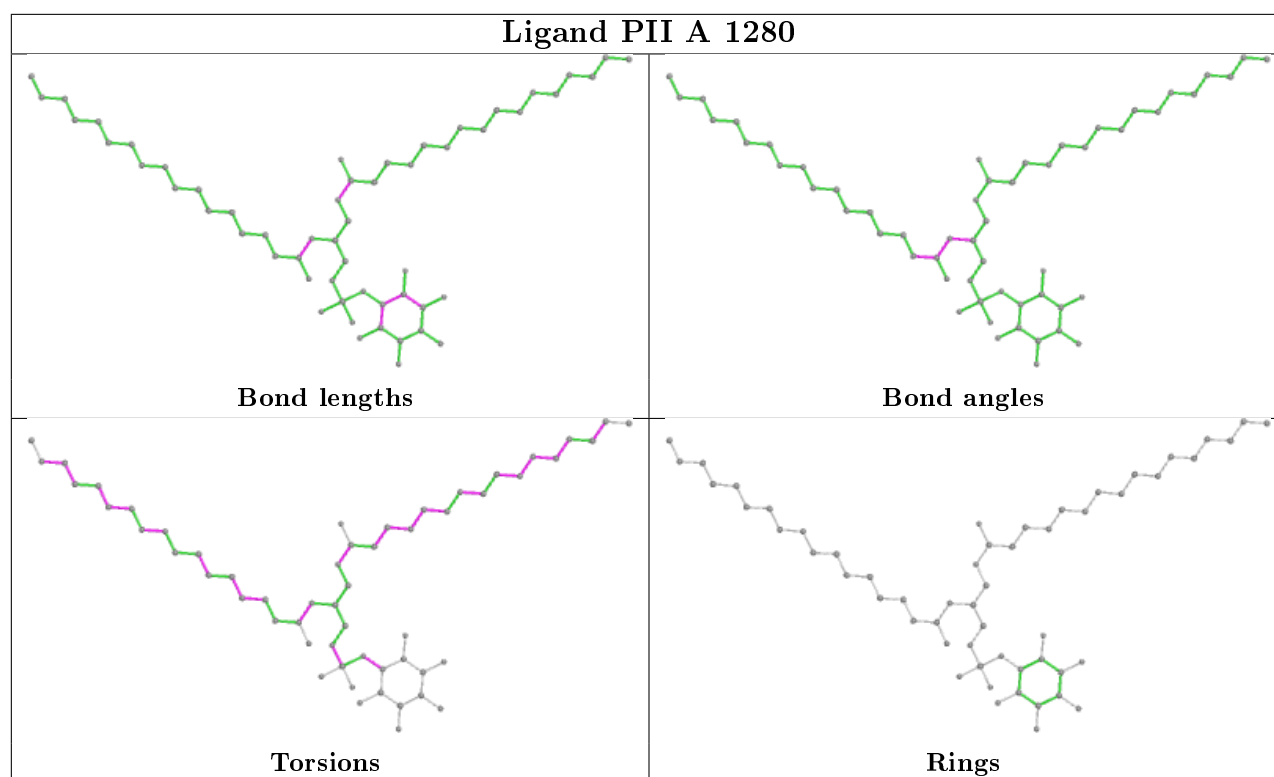
There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1284	D12	6	0
4	A	1283	NO3	1	0
4	A	1282	NO3	1	0
4	A	1281	NO3	1	0
6	A	1285	TWT	6	0
3	A	1280	PII	8	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	278/300 (92%)	-0.03	11 (3%) 38 40	34, 52, 85, 99	0
2	B	100/100 (100%)	-0.01	3 (3%) 50 53	37, 62, 93, 111	0
All	All	378/400 (94%)	-0.03	14 (3%) 41 44	34, 53, 89, 111	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	6.7
1	A	199	PRO	3.8
1	A	89	GLN	3.1
2	B	74	GLU	3.0
2	B	48	LYS	2.8
1	A	12	VAL	2.7
1	A	152	GLN	2.6
1	A	77	PHE	2.6
1	A	106	SER	2.4
1	A	198	GLY	2.2
2	B	18	GLY	2.2
1	A	84	PHE	2.1
1	A	200	GLY	2.1
1	A	13	ILE	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

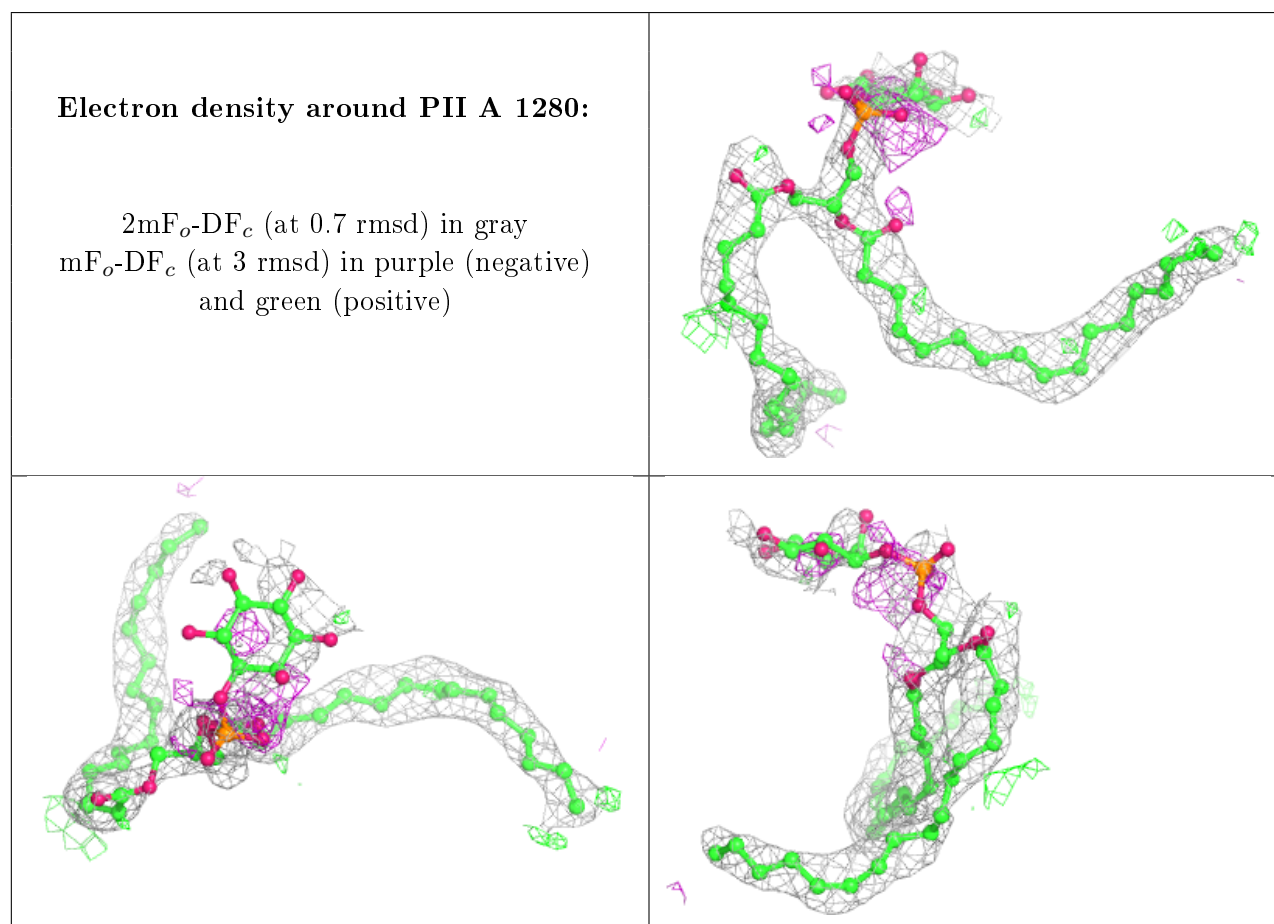
There are no carbohydrates in this entry.

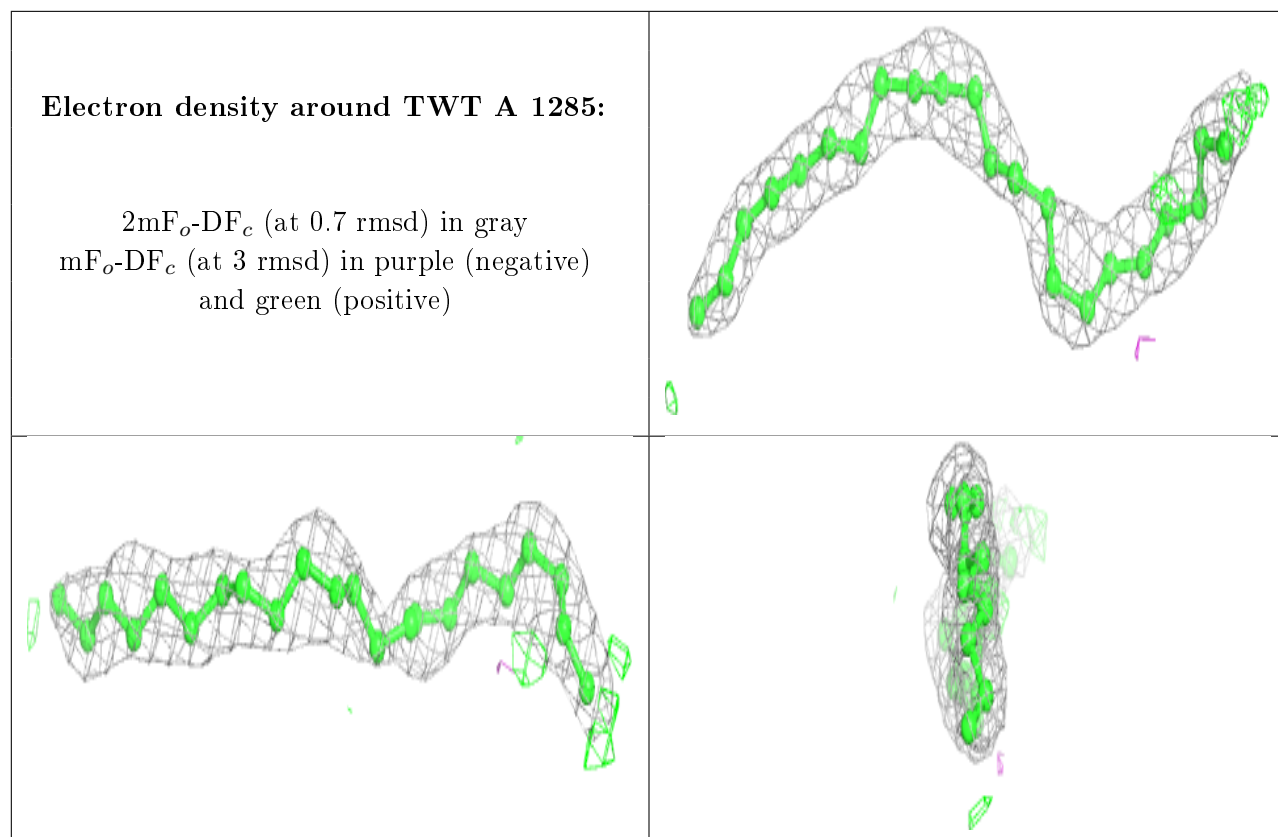
## 6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PII	A	1280	56/56	0.31	0.48	51,94,152,153	0
4	NO3	A	1282	4/4	0.41	0.32	80,86,86,90	0
5	D12	A	1284	12/12	0.85	0.19	63,70,83,86	0
4	NO3	A	1283	4/4	0.88	0.17	88,89,89,90	0
6	TWT	A	1285	22/22	0.91	0.48	51,62,69,70	0
4	NO3	A	1281	4/4	0.95	0.23	64,67,70,72	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.