Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2020 – 11:08 AM BST

PDB ID	:	6YZT
Title	:	Closo-carborane propyl-sulfonamide in complex with CA II
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Deposited on	:	2020-05-07
Resolution	:	1.05 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 following versions of software and data (see references ⓘ) were used in the production of this report:

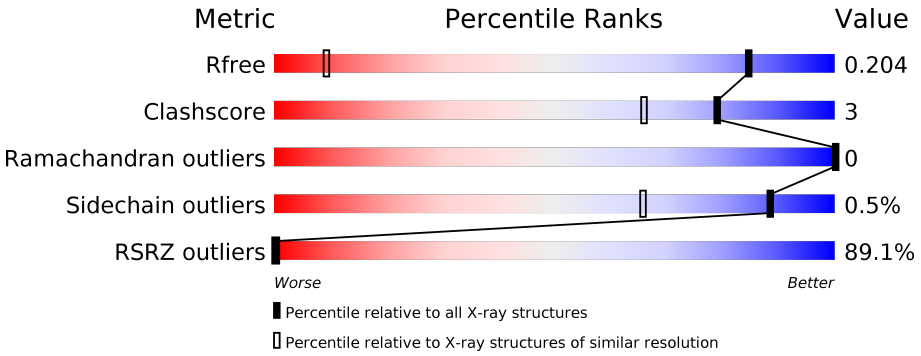
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.05 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	1202 (1.10-1.02)
Clashscore	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	260	88% 92% 6% ••

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	Q3E	A	302[A]	-	-	-	X
3	Q3E	A	302[B]	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2435 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.

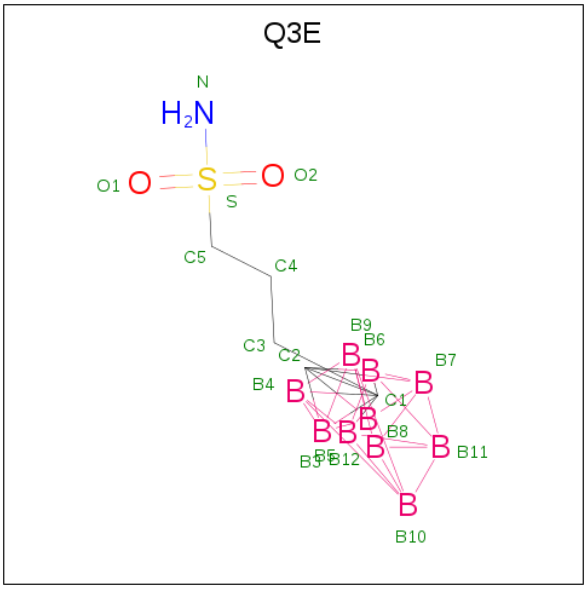
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	2131	1378	355	396	2	0	20	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- Molecule 3 is Carborane propyl-sulfonamide (three-letter code: Q3E) (formula: $C_5H_8B_{10}NO_2S$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	B	C	N	O	S		
3	A	1	38	20	10	2	4	2	0	1

- Molecule 4 is water.

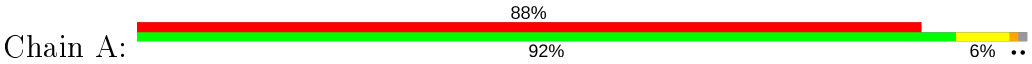
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	254	Total 265	O 265	0	11

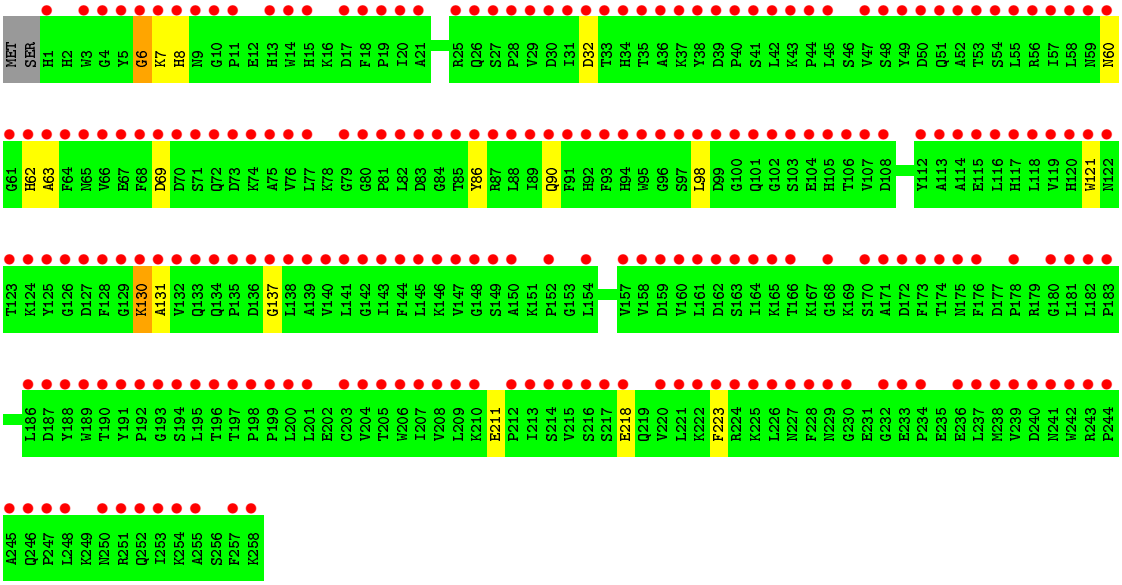
3 Residue-property plots (i)

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: Carbonic anhydrase 2

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.20Å 41.50Å 72.44Å 90.00° 104.56° 90.00°	Depositor
Resolution (Å)	40.84 – 1.05 40.84 – 1.05	Depositor EDS
% Data completeness (in resolution range)	94.5 (40.84-1.05) 94.5 (40.84-1.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.05Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.176 , 0.208 0.178 , 0.204	Depositor DCC
R_{free} test set	1068 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	10.0	Xtriage
Anisotropy	0.855	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2435	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, Q3E

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	0.90	3/2263 (0.1%)	0.96	8/3077 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	GLU	CD-OE2	13.80	1.40	1.25
1	A	121	TRP	CE3-CZ3	6.26	1.49	1.38
1	A	121	TRP	CG-CD2	-5.72	1.33	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	TYR	CB-CG-CD1	5.48	124.29	121.00
1	A	130	LYS	CD-CE-NZ	-5.37	99.35	111.70
1	A	69[A]	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	69[B]	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	223	PHE	CB-CG-CD2	-5.15	117.20	120.80
1	A	218	GLU	OE1-CD-OE2	-5.10	117.18	123.30
1	A	6	GLY	O-C-N	-5.08	114.57	122.70
1	A	218	GLU	CG-CD-OE1	5.03	128.35	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	6	GLY	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	2131	0	2077	12	0
2	A	1	0	0	0	0
3	A	38	0	0	0	0
4	A	265	0	0	4	0
All	All	2435	0	2077	12	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 3.

All (12) 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:A:32[A]:ASP:OD1	4:A:402:HOH:O	1.87	0.91
1:A:60:ASN:HD21	1:A:62[B]:HIS:CE1	1.95	0.84
1:A:211:GLU:OE2	4:A:424[B]:HOH:O	2.04	0.75
1:A:62[B]:HIS:CD2	4:A:453:HOH:O	2.44	0.70
1:A:60:ASN:OD1	1:A:62[B]:HIS:ND1	2.38	0.55
1:A:62[B]:HIS:HD1	1:A:63:ALA:N	2.09	0.51
1:A:60:ASN:ND2	1:A:62[B]:HIS:CE1	2.75	0.48
1:A:130:LYS:HE2	4:A:613:HOH:O	2.16	0.45
1:A:131:ALA:O	1:A:137:GLY:HA3	2.18	0.43
1:A:62[B]:HIS:ND1	1:A:63:ALA:N	2.69	0.41
1:A:98[A]:LEU:HD23	1:A:98[A]:LEU:HA	1.91	0.41
1:A:7[B]:LYS:O	1:A:8[B]:HIS:HB2	2.20	0.41

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	276/260 (106%)	264 (96%)	12 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	236/225 (105%)	235 (100%)	1 (0%)	91 73

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	65	ASN

5.3.3 RNA

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	Q3E	A	302[A]	2	25,37,37	1.29	3 (12%)	81,134,134	1.87	16 (19%)
3	Q3E	A	302[B]	2	25,37,37	1.36	3 (12%)	81,134,134	2.12	16 (19%)

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	Q3E	A	302[A]	2	-	4/10/450/450	-
3	Q3E	A	302[B]	2	-	0/10/450/450	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[B]	Q3E	B4-C1	2.92	1.77	1.72
3	A	302[A]	Q3E	B4-C1	2.80	1.77	1.72
3	A	302[B]	Q3E	S-N	-2.69	1.53	1.59
3	A	302[A]	Q3E	S-N	-2.46	1.54	1.59
3	A	302[B]	Q3E	B5-C1	-2.32	1.67	1.72
3	A	302[A]	Q3E	B5-C1	-2.28	1.67	1.72

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302[B]	Q3E	B10-B4-C1	-7.36	99.32	105.37
3	A	302[A]	Q3E	B10-B4-C1	-6.44	100.07	105.37
3	A	302[B]	Q3E	B9-B4-C1	-6.21	100.26	105.37
3	A	302[B]	Q3E	O2-S-O1	-5.73	111.22	119.32
3	A	302[B]	Q3E	O2-S-C5	-5.59	98.98	107.84
3	A	302[A]	Q3E	B9-B4-C1	-5.00	101.26	105.37
3	A	302[A]	Q3E	B5-B4-C1	-4.92	55.81	58.73
3	A	302[B]	Q3E	B5-B4-C1	-4.90	55.82	58.73
3	A	302[B]	Q3E	B4-B5-C1	4.21	61.23	58.73
3	A	302[A]	Q3E	B5-C1-C3	-4.12	113.71	121.78
3	A	302[B]	Q3E	B11-B5-C1	-4.07	102.02	105.37
3	A	302[A]	Q3E	B4-B5-C1	3.87	61.03	58.73
3	A	302[A]	Q3E	O2-S-O1	-3.73	114.04	119.32
3	A	302[B]	Q3E	B11-B5-B6	-3.59	56.15	58.70
3	A	302[B]	Q3E	B3-C1-B6	3.16	116.23	112.96
3	A	302[A]	Q3E	B11-B5-C1	-2.92	102.97	105.37
3	A	302[B]	Q3E	B12-B7-B6	-2.92	102.51	107.52
3	A	302[A]	Q3E	B3-C1-B6	2.81	115.87	112.96
3	A	302[B]	Q3E	B4-C1-B6	2.68	115.80	113.57
3	A	302[A]	Q3E	B11-B5-B6	-2.67	56.81	58.70
3	A	302[A]	Q3E	B12-B7-B6	-2.65	102.97	107.52
3	A	302[A]	Q3E	B9-B12-B11	2.56	111.10	108.06
3	A	302[B]	Q3E	B4-B10-B11	2.55	110.89	107.92
3	A	302[B]	Q3E	B5-C1-B6	2.51	64.00	62.24
3	A	302[A]	Q3E	B4-B10-B11	2.46	110.78	107.92
3	A	302[B]	Q3E	B7-B8-C2	2.35	59.77	55.86
3	A	302[A]	Q3E	B4-C1-B6	2.22	115.42	113.57
3	A	302[A]	Q3E	B7-B8-C2	2.21	59.53	55.86
3	A	302[A]	Q3E	B4-C1-B3	-2.06	60.80	62.24
3	A	302[B]	Q3E	B5-B11-B10	-2.04	57.86	59.88
3	A	302[A]	Q3E	B4-C1-C3	-2.03	117.80	121.78
3	A	302[B]	Q3E	C4-C3-C1	2.01	119.22	115.88

There are no chirality outliers.

All (4) torsion outliers are listed below:

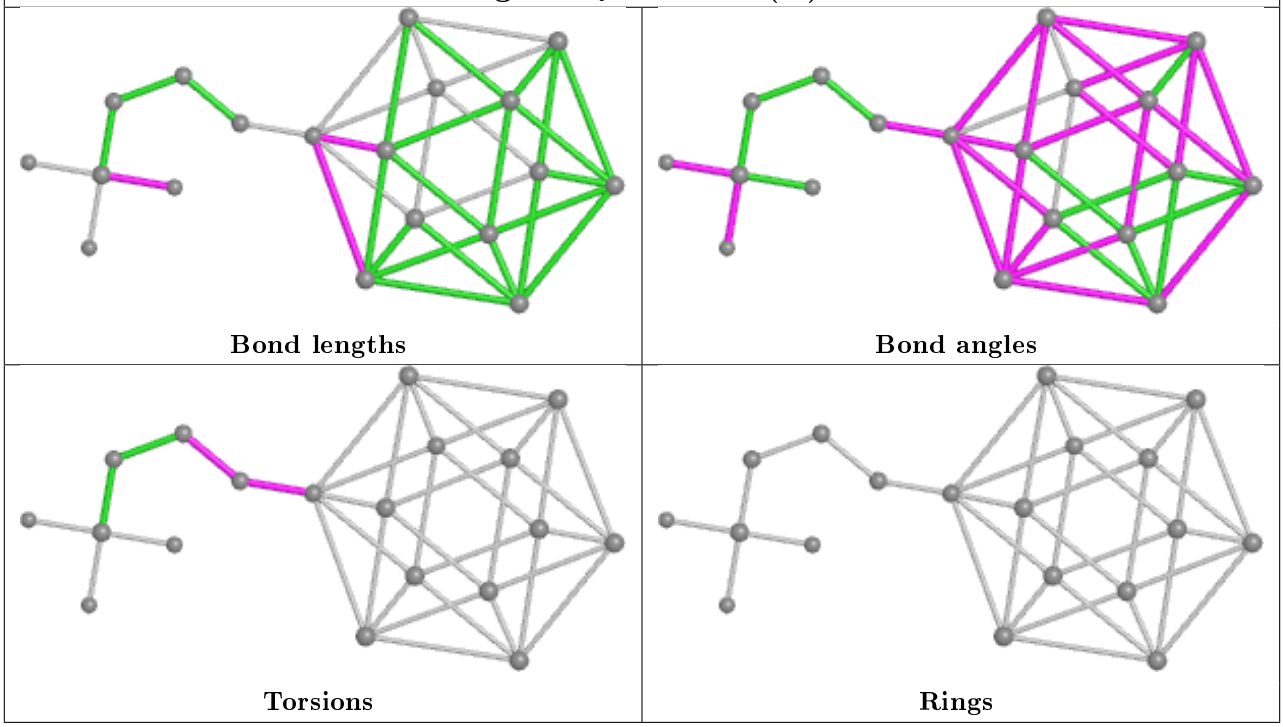
Mol	Chain	Res	Type	Atoms
3	A	302[A]	Q3E	B4-C1-C3-C4
3	A	302[A]	Q3E	C2-C1-C3-C4
3	A	302[A]	Q3E	C1-C3-C4-C5
3	A	302[A]	Q3E	B6-C1-C3-C4

There are no ring outliers.

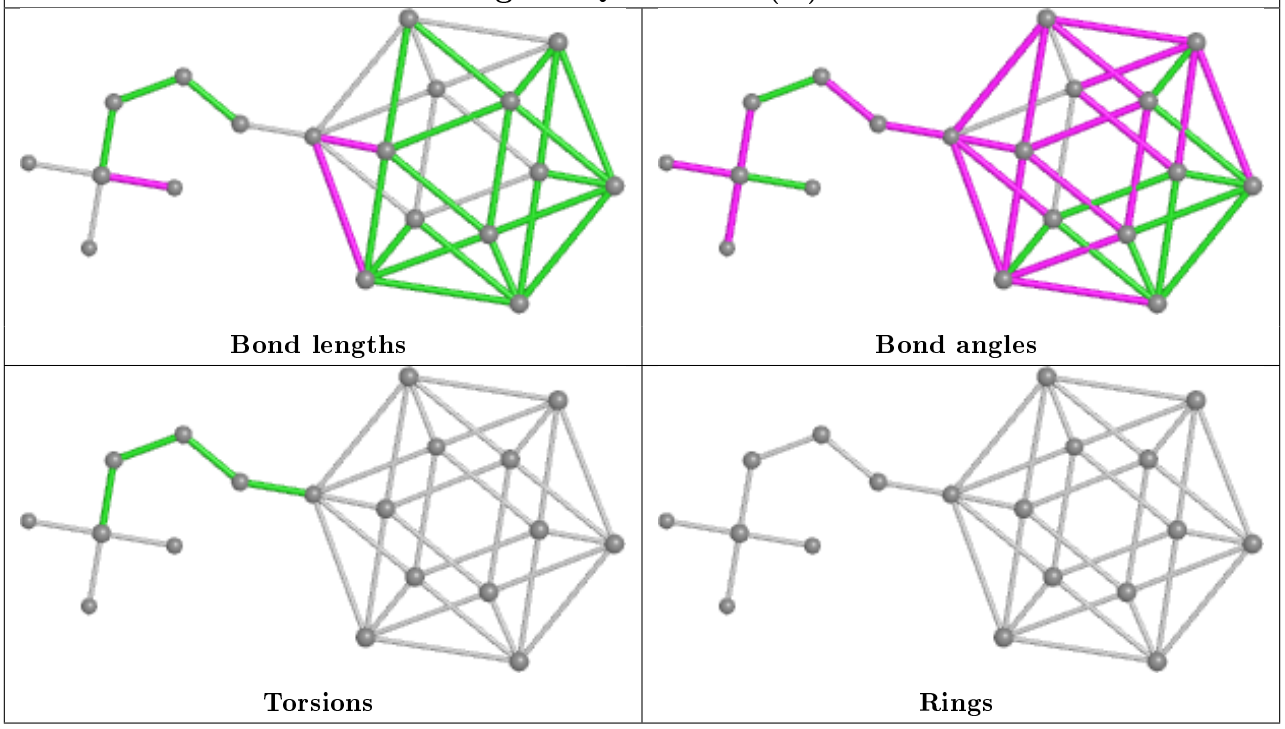
No monomer is involved in short contacts.

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 Q3E A 302 (A)



Ligand Q3E A 302 (B)



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, 95^{th} 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	258/260 (99%)	3.63	230 (89%)	0	0	11, 18, 30, 38	5 (1%)

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	TRP	9.1
1	A	143	ILE	7.5
1	A	207	ILE	7.0
1	A	95	TRP	6.9
1	A	45	LEU	6.5
1	A	242	TRP	6.4
1	A	128[A]	PHE	6.4
1	A	116	LEU	6.3
1	A	145	LEU	6.2
1	A	119	VAL	6.2
1	A	138[A]	LEU	6.1
1	A	206	TRP	6.1
1	A	139	ALA	6.0
1	A	64	PHE	6.0
1	A	189	TRP	6.0
1	A	140	VAL	5.9
1	A	203	CYS	5.9
1	A	258	LYS	5.9
1	A	1	HIS	5.9
1	A	91	PHE	5.7
1	A	68	PHE	5.6
1	A	208	VAL	5.6
1	A	85[A]	THR	5.6
1	A	38	TYR	5.6
1	A	118	LEU	5.5
1	A	221	LEU	5.4
1	A	147	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	20[A]	ILE	5.4
1	A	250	ASN	5.4
1	A	8[A]	HIS	5.3
1	A	195	LEU	5.3
1	A	144	PHE	5.2
1	A	76	VAL	5.2
1	A	55	LEU	5.2
1	A	89	ILE	5.2
1	A	141	LEU	5.2
1	A	209	LEU	5.2
1	A	114	ALA	5.2
1	A	205	THR	5.1
1	A	58	LEU	5.1
1	A	191	TYR	5.1
1	A	47	VAL	5.1
1	A	204	VAL	5.0
1	A	215	VAL	5.0
1	A	255	ALA	4.9
1	A	44	PRO	4.9
1	A	107	VAL	4.9
1	A	93	PHE	4.9
1	A	182	LEU	4.9
1	A	186	LEU	4.9
1	A	82	LEU	4.9
1	A	98[A]	LEU	4.9
1	A	201	LEU	4.9
1	A	53	THR	4.8
1	A	228	PHE	4.8
1	A	200	LEU	4.8
1	A	29	VAL	4.8
1	A	86	TYR	4.8
1	A	161	LEU	4.7
1	A	123	THR	4.7
1	A	57	ILE	4.7
1	A	213	ILE	4.6
1	A	14	TRP	4.6
1	A	5	TYR	4.6
1	A	158	VAL	4.5
1	A	113	ALA	4.5
1	A	131	ALA	4.5
1	A	236	GLU	4.5
1	A	66	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	88	LEU	4.4
1	A	197	THR	4.4
1	A	69[A]	ASP	4.4
1	A	49	TYR	4.4
1	A	73	ASP	4.4
1	A	142	GLY	4.3
1	A	248	LEU	4.3
1	A	132	VAL	4.3
1	A	192	PRO	4.3
1	A	220	VAL	4.3
1	A	239	VAL	4.3
1	A	31	ILE	4.3
1	A	21	ALA	4.2
1	A	43	LYS	4.2
1	A	176	PHE	4.2
1	A	164	ILE	4.2
1	A	230	GLY	4.2
1	A	252	GLN	4.2
1	A	190	THR	4.2
1	A	106	THR	4.1
1	A	196	THR	4.1
1	A	96	GLY	4.1
1	A	188	TYR	4.1
1	A	36	ALA	4.0
1	A	225	LYS	4.0
1	A	3	TRP	4.0
1	A	245	ALA	4.0
1	A	125	TYR	3.9
1	A	77	LEU	3.9
1	A	226	LEU	3.9
1	A	34[A]	HIS	3.9
1	A	232	GLY	3.9
1	A	253	ILE	3.9
1	A	42	LEU	3.9
1	A	112	TYR	3.8
1	A	157	VAL	3.8
1	A	237	LEU	3.8
1	A	168	GLY	3.8
1	A	71	SER	3.8
1	A	223	PHE	3.8
1	A	28	PRO	3.8
1	A	102	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	257	PHE	3.8
1	A	6	GLY	3.8
1	A	41	SER	3.7
1	A	18	PHE	3.7
1	A	173	PHE	3.7
1	A	40	PRO	3.7
1	A	137	GLY	3.7
1	A	75	ALA	3.7
1	A	154	LEU	3.7
1	A	165	LYS	3.7
1	A	193	GLY	3.7
1	A	105	HIS	3.6
1	A	233	GLU	3.6
1	A	27	SER	3.6
1	A	227	ASN	3.6
1	A	117	HIS	3.6
1	A	74	LYS	3.6
1	A	135	PRO	3.5
1	A	103	SER	3.5
1	A	178	PRO	3.5
1	A	159	ASP	3.5
1	A	33	THR	3.5
1	A	126	GLY	3.5
1	A	94	HIS	3.5
1	A	83	ASP	3.5
1	A	162[A]	ASP	3.4
1	A	166	THR	3.4
1	A	194	SER	3.4
1	A	240	ASP	3.4
1	A	120	HIS	3.4
1	A	172	ASP	3.4
1	A	54	SER	3.4
1	A	92	HIS	3.3
1	A	181	LEU	3.3
1	A	183	PRO	3.3
1	A	100	GLY	3.3
1	A	212[A]	PRO	3.3
1	A	244[A]	PRO	3.3
1	A	241	ASN	3.2
1	A	62[A]	HIS	3.2
1	A	214[A]	SER	3.2
1	A	25	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	65	ASN	3.1
1	A	90	GLN	3.1
1	A	198	PRO	3.1
1	A	51	GLN	3.1
1	A	217[A]	SER	3.0
1	A	97	SER	3.0
1	A	199	PRO	3.0
1	A	243	ARG	3.0
1	A	39	ASP	3.0
1	A	17	ASP	2.9
1	A	7[A]	LYS	2.9
1	A	37	LYS	2.9
1	A	163	SER	2.9
1	A	124	LYS	2.9
1	A	180	GLY	2.9
1	A	50[A]	ASP	2.9
1	A	70	ASP	2.9
1	A	30	ASP	2.9
1	A	234	PRO	2.8
1	A	247	PRO	2.8
1	A	133	GLN	2.8
1	A	148	GLY	2.8
1	A	63	ALA	2.8
1	A	60	ASN	2.8
1	A	127	ASP	2.8
1	A	81	PRO	2.8
1	A	122	ASN	2.8
1	A	101	GLN	2.8
1	A	254	LYS	2.8
1	A	35	THR	2.7
1	A	87	ARG	2.7
1	A	238	MET	2.7
1	A	84	GLY	2.7
1	A	171	ALA	2.7
1	A	160	VAL	2.7
1	A	222	LYS	2.7
1	A	10	GLY	2.7
1	A	152	PRO	2.6
1	A	130	LYS	2.6
1	A	72	GLN	2.6
1	A	210	LYS	2.6
1	A	150	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	32[A]	ASP	2.6
1	A	59	ASN	2.6
1	A	4	GLY	2.6
1	A	251	ARG	2.5
1	A	134	GLN	2.5
1	A	15	HIS	2.5
1	A	104	GLU	2.5
1	A	129	GLY	2.5
1	A	229	ASN	2.5
1	A	13	HIS	2.5
1	A	170	SER	2.5
1	A	52	ALA	2.4
1	A	19	PRO	2.4
1	A	48	SER	2.4
1	A	56	ARG	2.4
1	A	187	ASP	2.3
1	A	175	ASN	2.3
1	A	216	SER	2.3
1	A	79	GLY	2.3
1	A	11	PRO	2.3
1	A	218	GLU	2.3
1	A	174	THR	2.3
1	A	26	GLN	2.3
1	A	149[A]	SER	2.2
1	A	224	ARG	2.2
1	A	108	ASP	2.2
1	A	115	GLU	2.2
1	A	136	ASP	2.2
1	A	80	GLY	2.2
1	A	9	ASN	2.2
1	A	246	GLN	2.2
1	A	61	GLY	2.1
1	A	67	GLU	2.1
1	A	146	LYS	2.0
1	A	99	ASP	2.0

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)

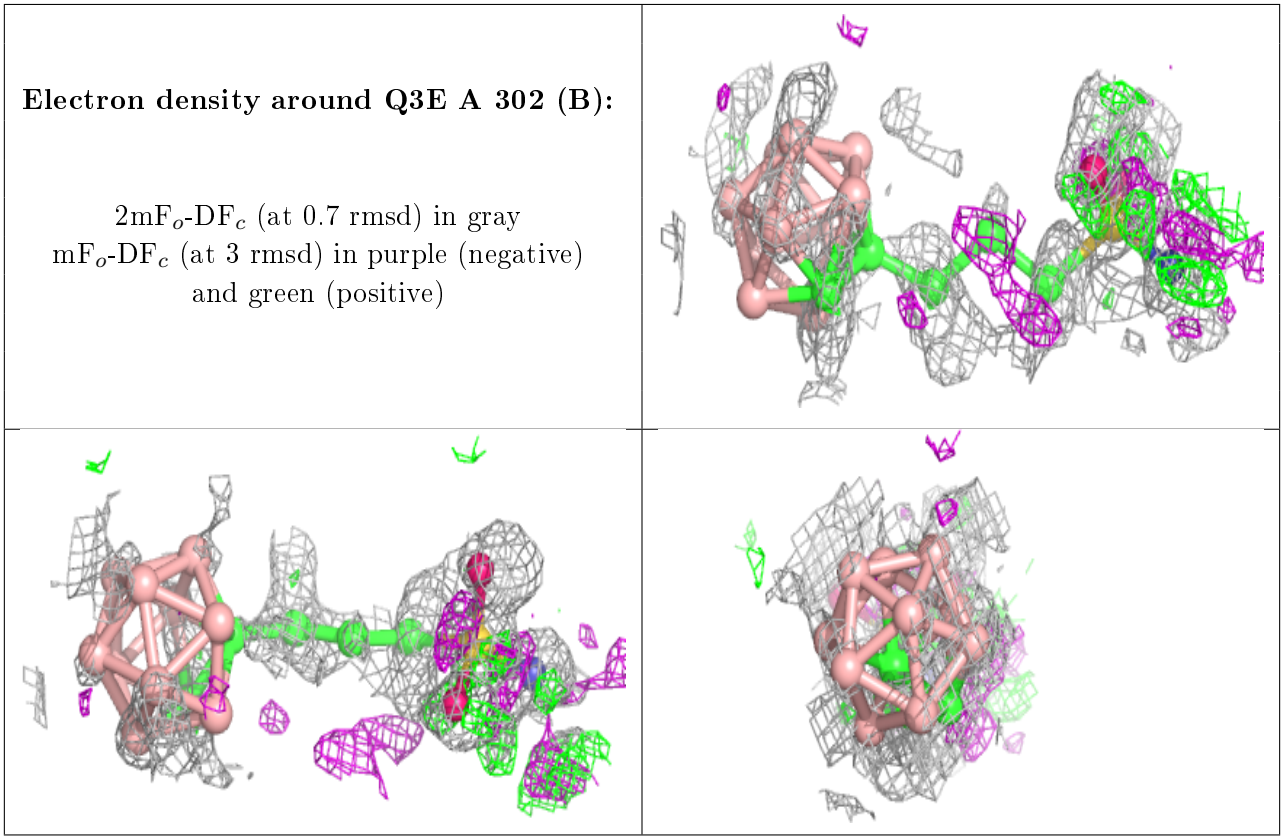
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	Q3E	A	302[B]	19/19	0.78	0.47	5,12,12,12	19
3	Q3E	A	302[A]	19/19	0.78	0.47	9,22,23,24	19
2	ZN	A	301	1/1	0.99	0.24	11,11,11,11	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.

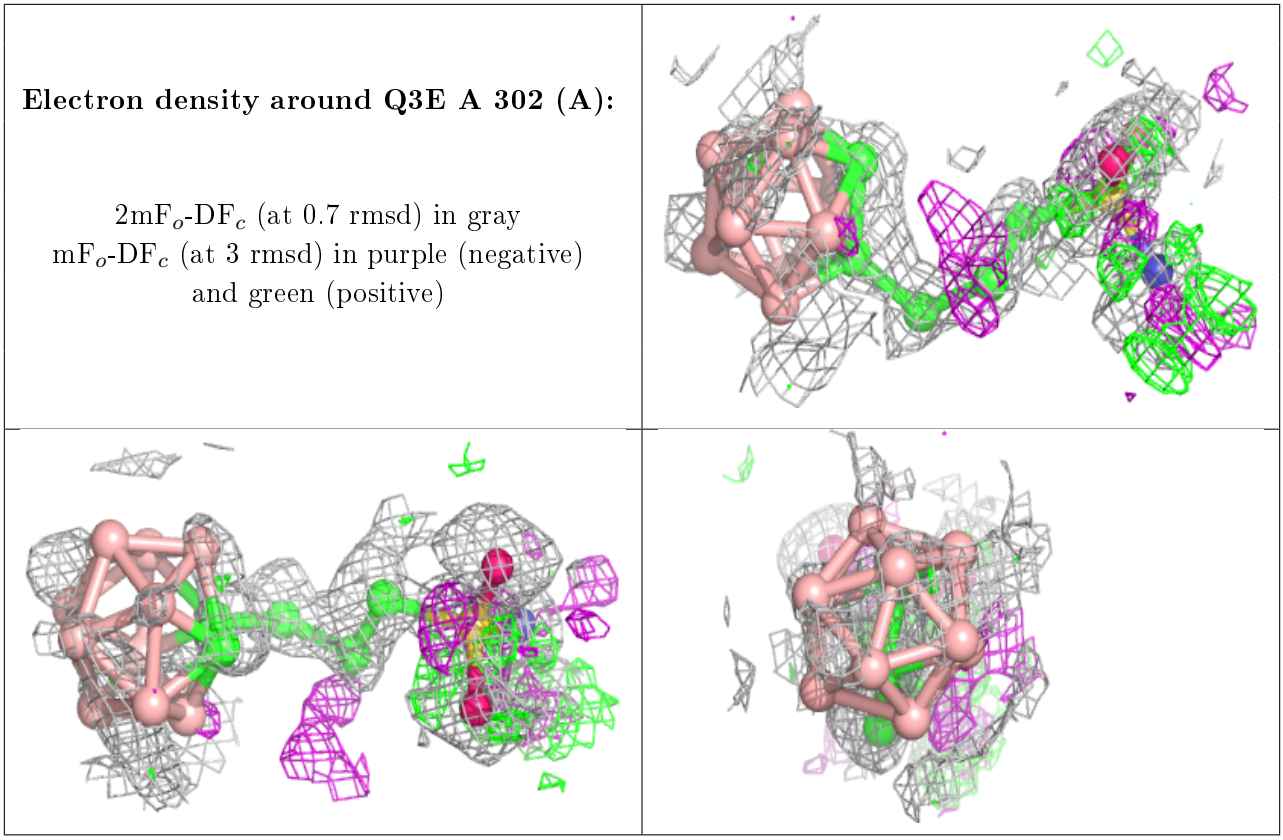
Electron density around Q3E A 302 (B):

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



Electron density around Q3E A 302 (A):

$2mF_o$-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.