



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:24 AM UTC

PDB ID : 3Q9Z / pdb_00003q9z
Title : Crystal structure of human CK2 alpha in complex with Quinalizarin at pH 6.5
Authors : Battistutta, R.; Ranchio, A.; Papinutto, E.
Deposited on : 2011-01-10
Resolution : 2.20 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

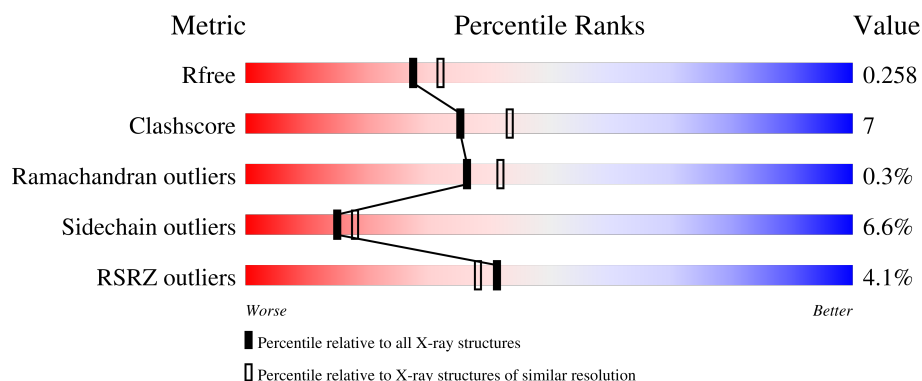
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	336	3% 83% 12% ..
1	B	336	5% 77% 18% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5981 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	1	0
			2809	1798	495	505	11			
1	B	332	Total	C	N	O	S	0	2	0
			2817	1803	498	505	11			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



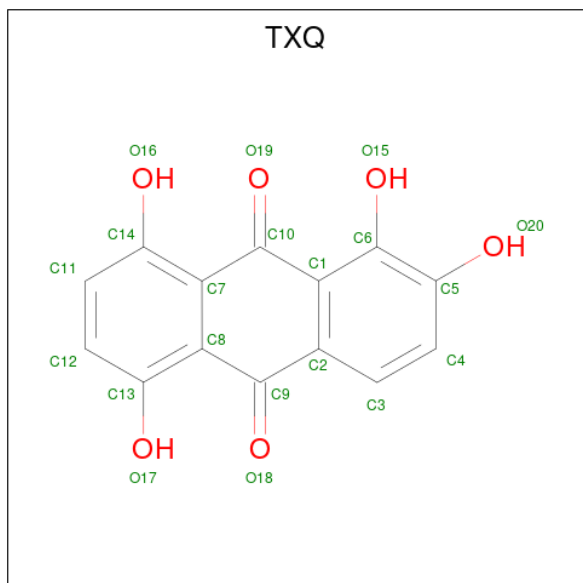
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2,5,8-tetrahydroxyanthracene-9,10-dione (CCD ID: TXQ) (formula: $C_{14}H_8O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

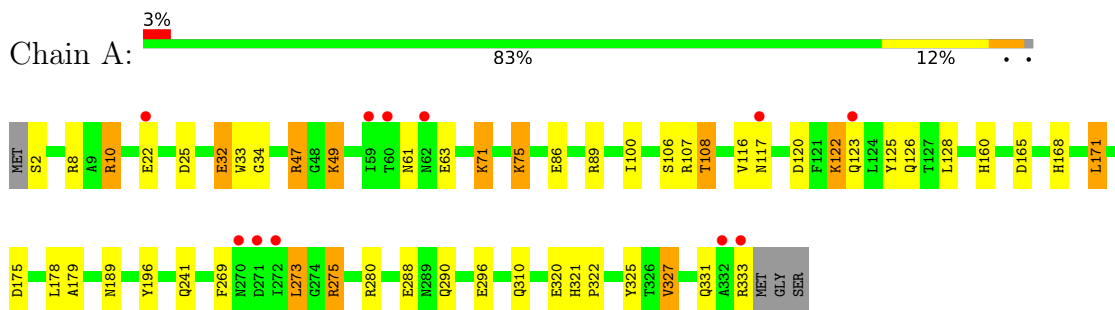
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	142	Total O 142 142	0	0
6	B	134	Total O 134 134	0	0

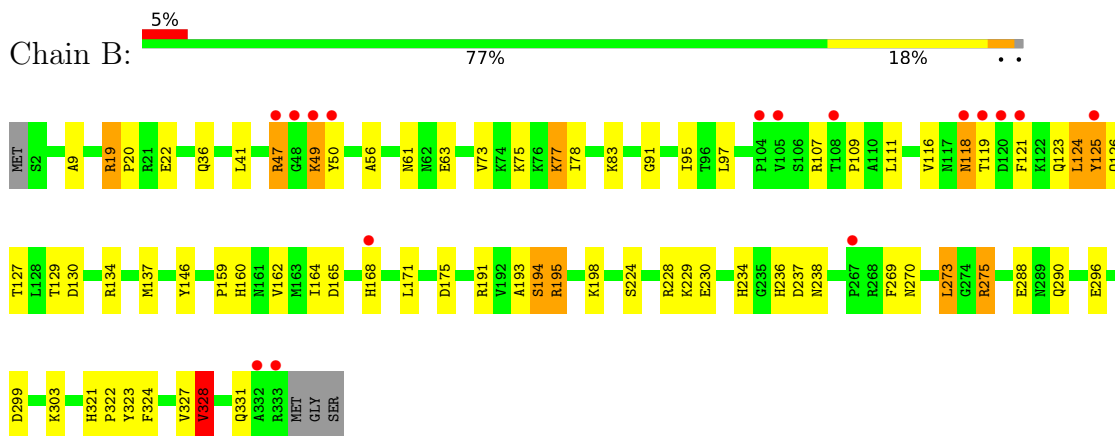
3 Residue-property plots [i](#)

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: Casein kinase II subunit alpha



- Molecule 1: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.96Å 127.96Å 125.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.22 – 2.20 57.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.8 (57.22-2.20) 94.8 (57.22-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.213 , 0.267 0.207 , 0.258	Depositor DCC
R_{free} test set	2564 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,-l,-k 0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5981	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TXQ, SO4, NA, EDO

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	1.27	3/2887 (0.1%)	1.16	9/3904 (0.2%)
1	B	1.28	4/2898 (0.1%)	1.17	8/3918 (0.2%)
All	All	1.27	7/5785 (0.1%)	1.16	17/7822 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	ILE	CA-CB	6.36	1.60	1.54
1	A	179	ALA	CA-CB	6.16	1.63	1.53
1	B	9	ALA	N-CA	5.83	1.53	1.46
1	B	328	VAL	CA-CB	5.83	1.61	1.54
1	A	325	TYR	N-CA	5.30	1.52	1.46
1	B	97	LEU	C-O	-5.26	1.17	1.24
1	A	32	GLU	C-O	-5.12	1.17	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	NE-CZ-NH2	9.04	127.34	119.20
1	A	280	ARG	NE-CZ-NH1	-8.15	113.35	121.50
1	B	19	ARG	CA-C-N	-6.79	112.79	119.78
1	B	19	ARG	C-N-CA	-6.79	112.79	119.78
1	B	175	ASP	N-CA-C	6.52	118.54	110.91
1	A	10	ARG	CD-NE-CZ	6.31	133.23	124.40
1	A	280	ARG	CD-NE-CZ	6.12	132.97	124.40
1	A	10	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	A	108	THR	N-CA-C	5.85	117.02	109.65
1	B	47	ARG	NE-CZ-NH1	-5.84	115.66	121.50
1	B	47	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	B	328	VAL	N-CA-CB	5.64	118.21	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	ARG	N-CA-C	5.49	122.50	110.80
1	A	175	ASP	N-CA-C	5.48	117.87	111.02
1	A	108	THR	CB-CA-C	5.28	117.96	109.41
1	A	171	LEU	CA-CB-CG	5.28	134.78	116.30
1	B	270	ASN	N-CA-C	5.07	117.19	111.11

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	2809	0	2752	36	0
1	B	2817	0	2765	48	0
2	A	15	0	0	2	0
2	B	15	0	0	1	0
3	A	20	0	6	0	0
3	B	20	0	6	2	0
4	A	8	0	12	3	0
5	B	1	0	0	0	0
6	A	142	0	0	10	0
6	B	134	0	0	4	0
All	All	5981	0	5541	83	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 7.

All (83) 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:B:121:PHE:CD1	1:B:164:ILE:HD11	1.80	1.16
1:B:121:PHE:HD1	1:B:164:ILE:CD1	1.60	1.14
1:B:121:PHE:CD1	1:B:164:ILE:CD1	2.32	1.12
1:B:121:PHE:CE1	1:B:164:ILE:HD11	1.98	0.98
1:B:234:HIS:CD2	6:B:374:HOH:O	2.21	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PHE:CD1	1:B:164:ILE:HD12	2.07	0.90
1:B:121:PHE:HD1	1:B:164:ILE:HD12	1.40	0.82
1:B:119:THR:HG21	6:B:429:HOH:O	1.78	0.81
1:A:320:GLU:HG3	6:A:374:HOH:O	1.81	0.80
1:B:50:TYR:HA	6:B:443:HOH:O	1.88	0.73
1:B:121:PHE:CE1	1:B:164:ILE:CD1	2.66	0.71
1:A:61:ASN:OD1	1:A:63:GLU:HB2	1.91	0.71
1:A:25:ASP:HA	4:A:341:EDO:C2	2.22	0.69
1:B:160:HIS:O	1:B:160:HIS:CD2	2.47	0.68
1:A:25:ASP:HA	4:A:341:EDO:H22	1.80	0.64
1:B:118:ASN:HD22	3:B:340:TXQ:H12	1.63	0.64
1:A:165:ASP:OD2	1:A:168:HIS:HD2	1.81	0.63
1:A:120:ASP:HB3	1:A:123:GLN:OE1	1.98	0.62
1:A:47:ARG:HD3	6:A:483:HOH:O	2.01	0.61
1:B:119:THR:HG23	1:B:123:GLN:HG3	1.83	0.61
1:B:118:ASN:ND2	3:B:340:TXQ:H12	2.16	0.60
1:A:86:GLU:HG2	1:A:89:ARG:HH22	1.67	0.59
1:A:47:ARG:CD	6:A:483:HOH:O	2.51	0.58
1:A:34:GLY:HA3	6:A:359:HOH:O	2.03	0.57
1:A:89:ARG:NH2	1:B:236:HIS:HB3	2.19	0.57
1:A:106:SER:O	1:A:107:ARG:HB2	2.05	0.57
1:B:49:LYS:HB3	1:B:50:TYR:HD1	1.69	0.56
1:B:73:VAL:HG21	1:B:77:LYS:HG2	1.87	0.56
1:A:71:LYS:HE3	6:A:483:HOH:O	2.06	0.55
1:A:86:GLU:HG2	1:A:89:ARG:NH2	2.23	0.54
1:B:160:HIS:CD2	1:B:160:HIS:C	2.86	0.54
1:B:125:TYR:OH	1:B:230:GLU:HG3	2.09	0.53
1:A:327:VAL:O	1:A:331:GLN:HG3	2.09	0.53
1:A:327:VAL:HG13	6:A:349:HOH:O	2.09	0.52
1:B:61:ASN:OD1	1:B:63:GLU:HB2	2.10	0.52
1:B:73:VAL:HG21	1:B:77:LYS:HE3	1.91	0.51
1:A:33:TRP:CE3	1:A:100:ILE:HG22	2.46	0.51
1:B:198:LYS:HE3	1:B:238:ASN:OD1	2.10	0.50
1:A:75:LYS:NZ	2:A:338:SO4:O1	2.40	0.50
1:B:165:ASP:OD2	1:B:168:HIS:HD2	1.94	0.50
1:B:121:PHE:HB3	1:B:159:PRO:O	2.12	0.49
1:B:321:HIS:CG	1:B:322:PRO:HD2	2.47	0.49
1:A:120:ASP:OD2	1:A:122:LYS:HB2	2.13	0.49
1:A:71:LYS:CE	6:A:483:HOH:O	2.61	0.49
1:B:49:LYS:C	1:B:50:TYR:CD1	2.91	0.49
1:B:324:PHE:O	1:B:328:VAL:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PHE:HB2	1:B:162:VAL:HB	1.94	0.48
1:B:49:LYS:C	1:B:50:TYR:HD1	2.22	0.48
1:A:71:LYS:NZ	6:A:483:HOH:O	2.39	0.48
1:B:49:LYS:HB3	1:B:50:TYR:CD1	2.49	0.47
1:A:269:PHE:HB3	1:A:273:LEU:HD22	1.97	0.47
1:B:78:ILE:HD13	1:B:109:PRO:HG2	1.96	0.47
1:A:333:ARG:O	1:A:333:ARG:HD3	2.15	0.46
1:A:34:GLY:CA	6:A:359:HOH:O	2.62	0.46
1:A:189:ASN:ND2	2:A:337:SO4:O4	2.49	0.46
1:A:160:HIS:O	1:A:160:HIS:CD2	2.68	0.46
1:B:91:GLY:HA3	1:B:146:TYR:CE2	2.51	0.46
1:B:191:ARG:NE	2:B:338:SO4:O1	2.49	0.45
1:B:299:ASP:OD2	1:B:303:LYS:HE2	2.17	0.45
1:A:33:TRP:CZ3	1:A:100:ILE:HG22	2.51	0.45
1:B:124:LEU:C	1:B:126:GLN:H	2.25	0.45
1:B:134:ARG:HG2	1:B:323:TYR:CZ	2.52	0.45
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.73	0.45
1:A:25:ASP:HA	4:A:341:EDO:H21	1.99	0.44
1:A:321:HIS:CG	1:A:322:PRO:HD2	2.51	0.44
1:A:196:TYR:HA	1:A:241:GLN:NE2	2.33	0.44
1:A:10:ARG:HD3	1:A:310:GLN:O	2.19	0.43
1:B:129:THR:O	1:B:130:ASP:C	2.61	0.43
1:B:237:ASP:OD1	1:B:237:ASP:C	2.61	0.43
1:B:19:ARG:O	1:B:20:PRO:C	2.59	0.42
1:B:47:ARG:HD3	6:B:442:HOH:O	2.19	0.42
1:B:224:SER:HB2	1:B:229:LYS:O	2.19	0.42
1:B:269:PHE:HB3	1:B:273:LEU:HD22	2.01	0.42
1:B:41:LEU:HD23	1:B:56:ALA:HB2	2.01	0.41
1:A:160:HIS:CD2	1:A:160:HIS:C	2.98	0.41
1:A:125:TYR:HA	1:A:128:LEU:HD12	2.01	0.41
1:B:275:ARG:HE	1:B:275:ARG:HB2	1.44	0.41
1:B:22:GLU:O	1:B:83:LYS:HE2	2.19	0.41
1:A:63:GLU:OE1	6:A:481:HOH:O	2.22	0.41
1:B:137:MET:HE3	1:B:137:MET:HB3	1.79	0.41
1:A:275:ARG:HE	1:A:275:ARG:HB2	1.48	0.40
1:A:49:LYS:HD2	1:A:178:LEU:HD11	2.03	0.40
1:B:194:SER:O	1:B:195:ARG:C	2.64	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	331/336 (98%)	313 (95%)	18 (5%)	0	100	100
1	B	332/336 (99%)	310 (93%)	20 (6%)	2 (1%)	21	23
All	All	663/672 (99%)	623 (94%)	38 (6%)	2 (0%)	36	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	ALA
1	B	118	ASN

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	306/308 (99%)	286 (94%)	20 (6%)	15	18
1	B	307/308 (100%)	287 (94%)	20 (6%)	15	18
All	All	613/616 (100%)	573 (94%)	40 (6%)	15	18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	8	ARG
1	A	22	GLU
1	A	32	GLU

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Mol	Chain	Res	Type
1	A	47	ARG
1	A	49	LYS
1	A	71	LYS
1	A	75	LYS
1	A	108	THR
1	A	116	VAL
1	A	117	ASN
1	A	122	LYS
1	A	126	GLN
1	A	171	LEU
1	A	273	LEU
1	A	275	ARG
1	A	288	GLU
1	A	290	GLN
1	A	296	GLU
1	A	327	VAL
1	B	36	GLN
1	B	49	LYS
1	B	75	LYS
1	B	77	LYS
1	B	107	ARG
1	B	116	VAL
1	B	124	LEU
1	B	125	TYR
1	B	127	THR
1	B	171	LEU
1	B	194	SER
1	B	228	ARG
1	B	273	LEU
1	B	275	ARG
1	B	288	GLU
1	B	290	GLN
1	B	296	GLU
1	B	327	VAL
1	B	328	VAL
1	B	331	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	160	HIS

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Mol	Chain	Res	Type
1	A	168	HIS
1	A	186	GLN
1	A	207	GLN
1	A	331	GLN
1	B	118	ASN
1	B	160	HIS
1	B	168	HIS
1	B	207	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z > 2$
2	SO4	A	337	-	4,4,4	0.47	0	6,6,6	0.74	0
2	SO4	B	338	-	4,4,4	0.25	0	6,6,6	0.42	0
3	TXQ	B	340	-	22,22,22	1.27	3 (13%)	34,34,34	1.04	2 (5%)
2	SO4	A	338	-	4,4,4	0.17	0	6,6,6	0.27	0
2	SO4	A	339	-	4,4,4	0.43	0	6,6,6	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TXQ	A	340	-	22,22,22	1.34	3 (13%)	34,34,34	1.34	3 (8%)
2	SO4	B	339	-	4,4,4	0.41	0	6,6,6	0.54	0
2	SO4	B	337	-	4,4,4	0.31	0	6,6,6	0.78	0
4	EDO	A	342	-	3,3,3	0.52	0	2,2,2	0.29	0
4	EDO	A	341	-	3,3,3	0.32	0	2,2,2	0.82	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	TXQ	A	340	-	-	-	0/3/3/3
3	TXQ	B	340	-	-	-	0/3/3/3
4	EDO	A	342	-	-	1/1/1/1	-
4	EDO	A	341	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	340	TXQ	O18-C9	3.03	1.28	1.22
3	A	340	TXQ	O19-C10	2.49	1.27	1.22
3	B	340	TXQ	C4-C3	2.49	1.42	1.38
3	B	340	TXQ	O18-C9	2.25	1.26	1.22
3	A	340	TXQ	C1-C6	-2.15	1.37	1.41
3	B	340	TXQ	C2-C1	-2.11	1.38	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	340	TXQ	C4-C5-C6	2.87	123.06	120.09
3	A	340	TXQ	C3-C4-C5	-2.61	117.89	120.50
3	B	340	TXQ	C11-C12-C13	-2.39	118.11	120.50
3	B	340	TXQ	C3-C4-C5	-2.22	118.28	120.50
3	A	340	TXQ	O16-C14-C7	-2.01	117.42	121.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	341	EDO	O1-C1-C2-O2

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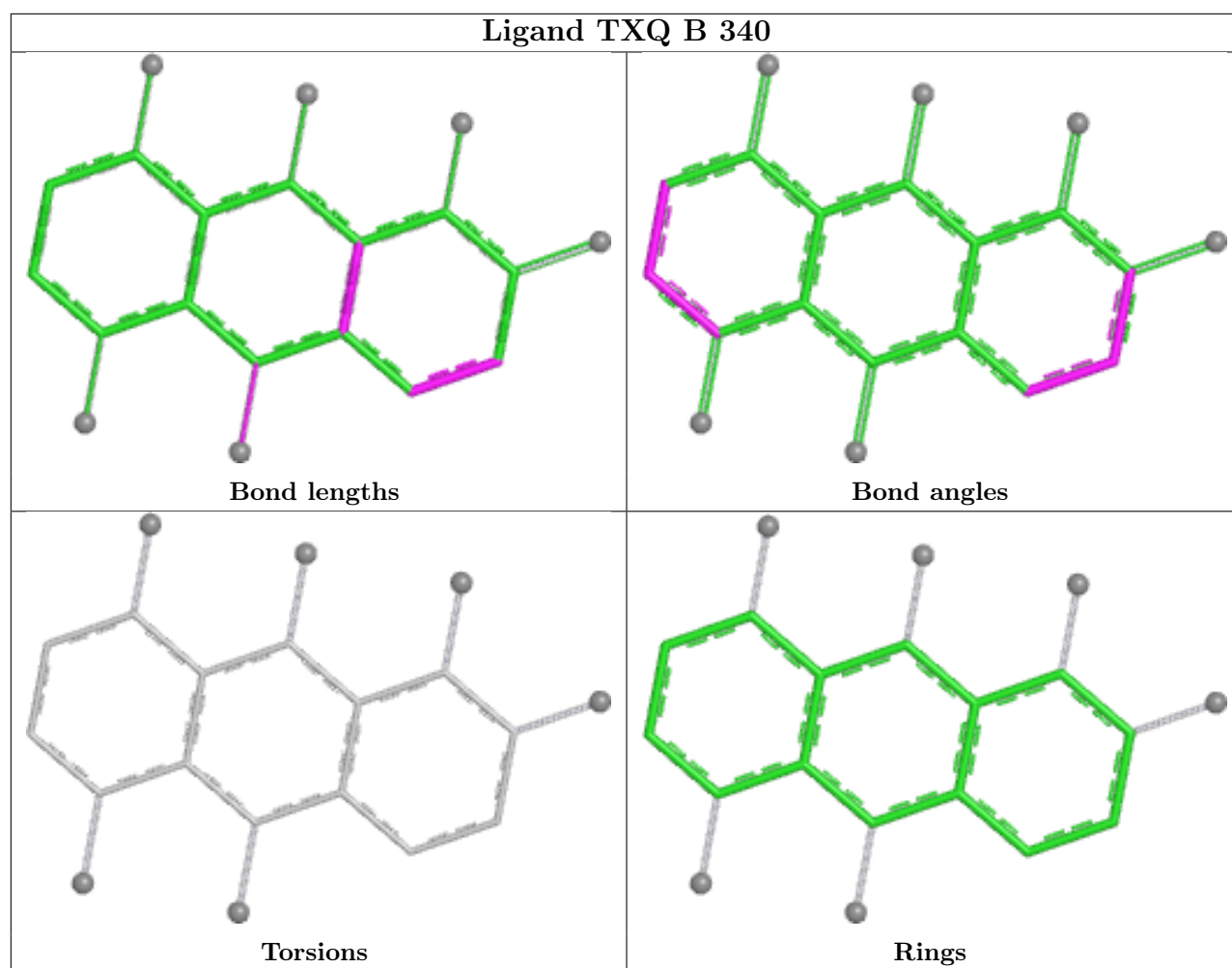
Mol	Chain	Res	Type	Atoms
4	A	342	EDO	O1-C1-C2-O2

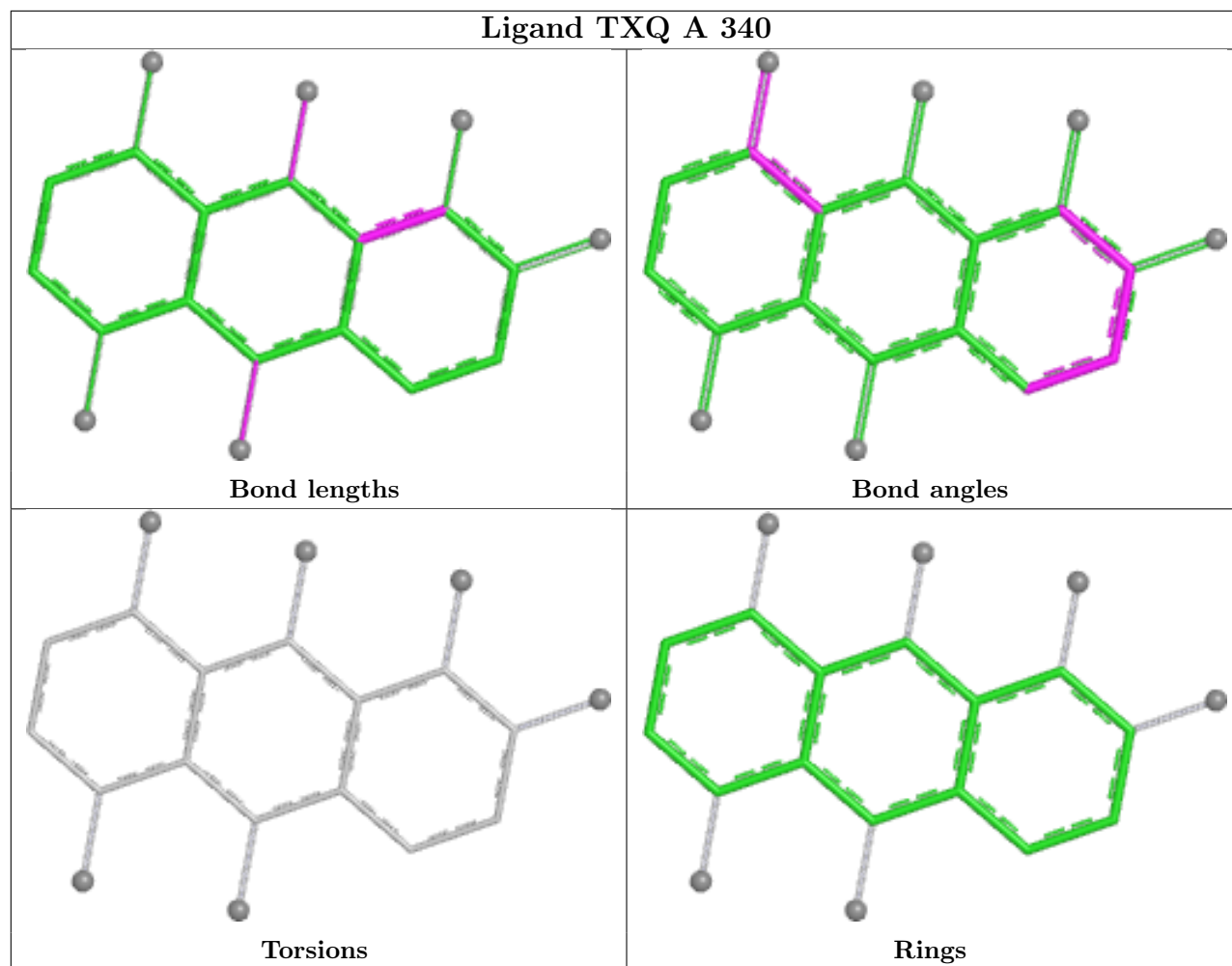
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	337	SO4	1	0
2	B	338	SO4	1	0
3	B	340	TXQ	2	0
2	A	338	SO4	1	0
4	A	341	EDO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	332/336 (98%)	0.14	11 (3%)	49 46	26, 41, 67, 92	1 (0%)
1	B	332/336 (98%)	0.25	16 (4%)	35 32	21, 41, 70, 100	2 (0%)
All	All	664/672 (98%)	0.19	27 (4%)	41 38	21, 41, 69, 100	3 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	ALA	6.7
1	B	332	ALA	5.6
1	A	60	THR	5.0
1	B	105	VAL	4.0
1	A	333	ARG	3.2
1	B	121	PHE	3.1
1	B	48	GLY	3.1
1	B	119	THR	3.0
1	A	271	ASP	2.9
1	B	108	THR	2.9
1	A	117	ASN	2.7
1	A	62	ASN	2.6
1	B	120	ASP	2.6
1	A	272	ILE	2.6
1	A	123	GLN	2.4
1	B	333	ARG	2.4
1	B	267	PRO	2.3
1	B	168	HIS	2.3
1	B	118	ASN	2.3
1	B	47	ARG	2.3
1	B	125	TYR	2.3
1	A	22	GLU	2.2
1	B	104	PRO	2.2
1	B	50	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	59	ILE	2.1
1	A	270	ASN	2.1
1	B	49	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

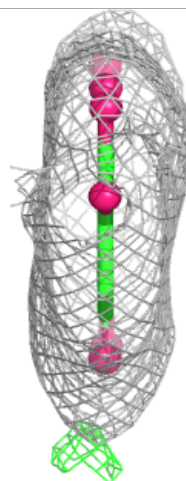
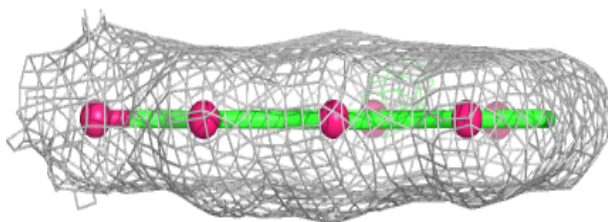
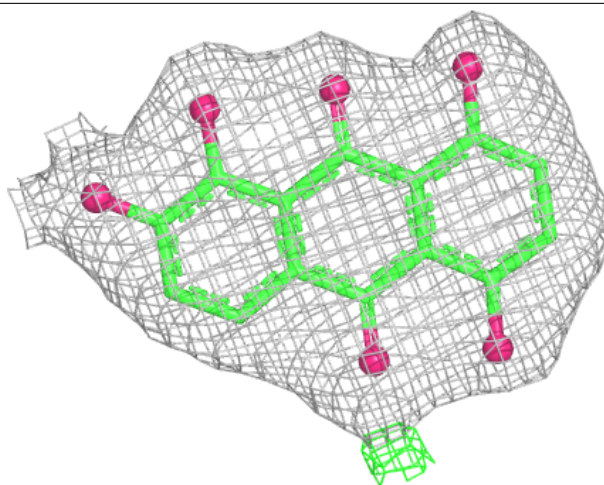
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

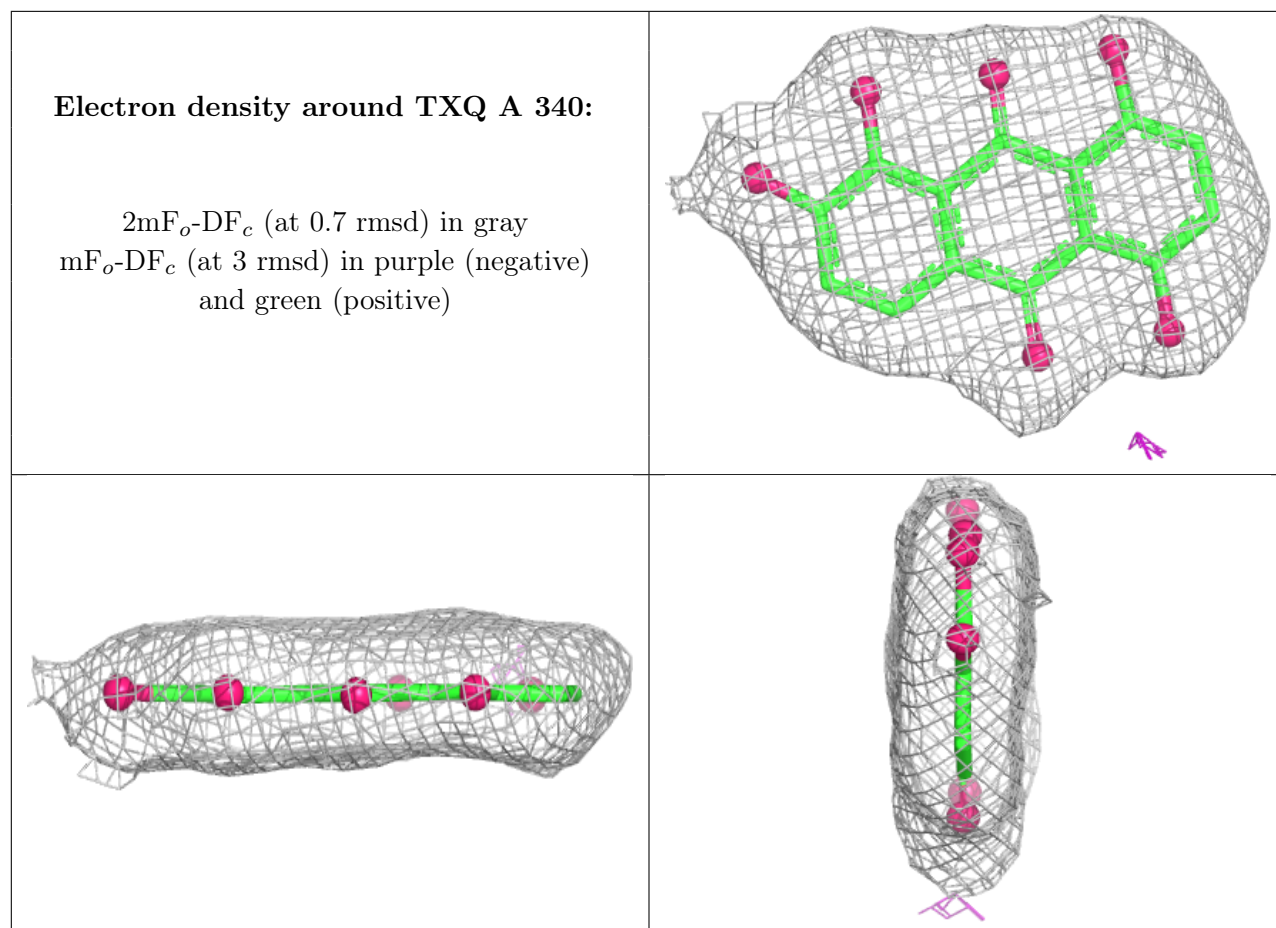
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NA	B	341	1/1	0.78	0.20	64,64,64,64	0
4	EDO	A	342	4/4	0.80	0.21	71,72,72,73	0
2	SO4	B	338	5/5	0.82	0.12	96,98,98,98	0
2	SO4	B	337	5/5	0.90	0.12	59,63,64,65	0
2	SO4	A	338	5/5	0.91	0.07	80,80,82,82	0
2	SO4	B	339	5/5	0.91	0.12	58,59,62,64	0
2	SO4	A	339	5/5	0.92	0.22	62,62,64,65	0
2	SO4	A	337	5/5	0.93	0.12	60,61,62,64	0
4	EDO	A	341	4/4	0.94	0.10	42,49,49,52	0
3	TXQ	B	340	20/20	0.95	0.06	30,36,39,39	0
3	TXQ	A	340	20/20	0.96	0.06	28,36,41,45	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 TXQ B 340:

$2mF_o-DF_c$ (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.