



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:25 pm BST

PDB ID : 3Q9X  
Title : Crystal structure of human CK2 alpha in complex with emodin 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](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

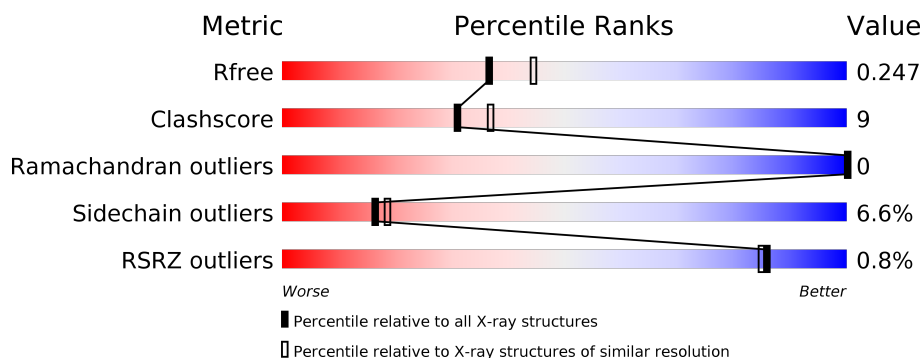
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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	336	
1	B	336	

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
4	7PE	A	338	-	-	X	-
5	SO4	B	341	-	-	X	-

## 2 Entry composition [i](#)

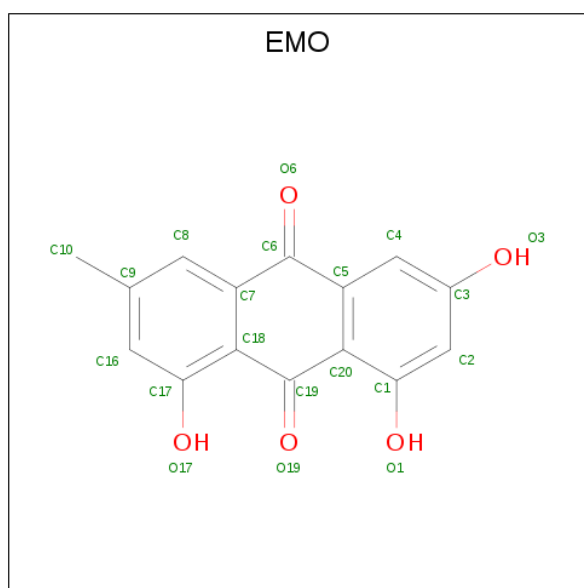
There are 7 unique types of molecules in this entry. The entry contains 5958 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	330	Total	C	N	O	S	0	3	0
			2812	1800	497	504	11			
1	B	330	Total	C	N	O	S	0	0	0
			2788	1786	490	501	11			

- Molecule 2 is 3-METHYL-1,6,8-TRIHIDROXYANTHRAQUINONE (three-letter code: EMO) (formula: C<sub>15</sub>H<sub>10</sub>O<sub>5</sub>).



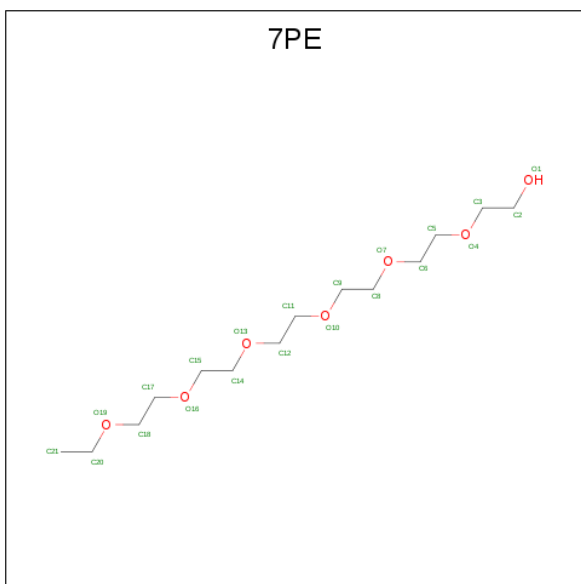
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	15	5		
2	B	1	Total	C	O	0	0
			20	15	5		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 4 is 2-(2-(2-(2-(2-(2-ETHOXYETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHANOL (three-letter code: 7PE) (formula: C<sub>14</sub>H<sub>30</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	14	7		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		

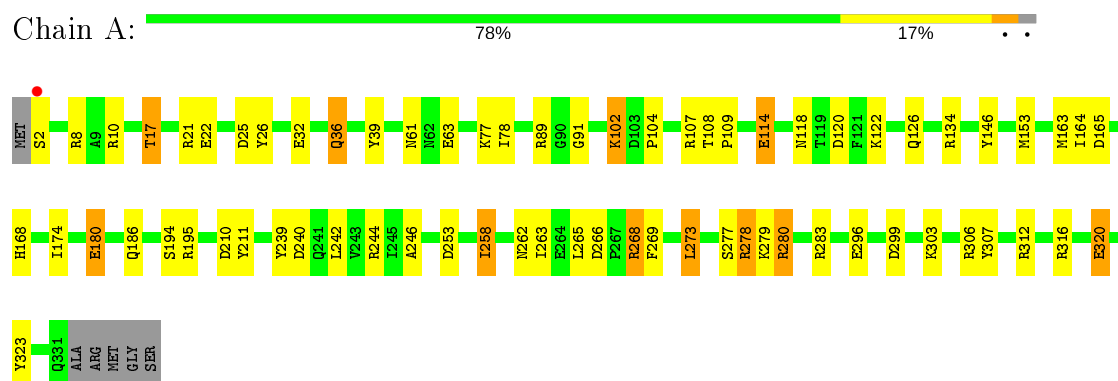
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	116	Total	O	0	0
			116	116		
7	B	131	Total	O	0	0
			131	131		

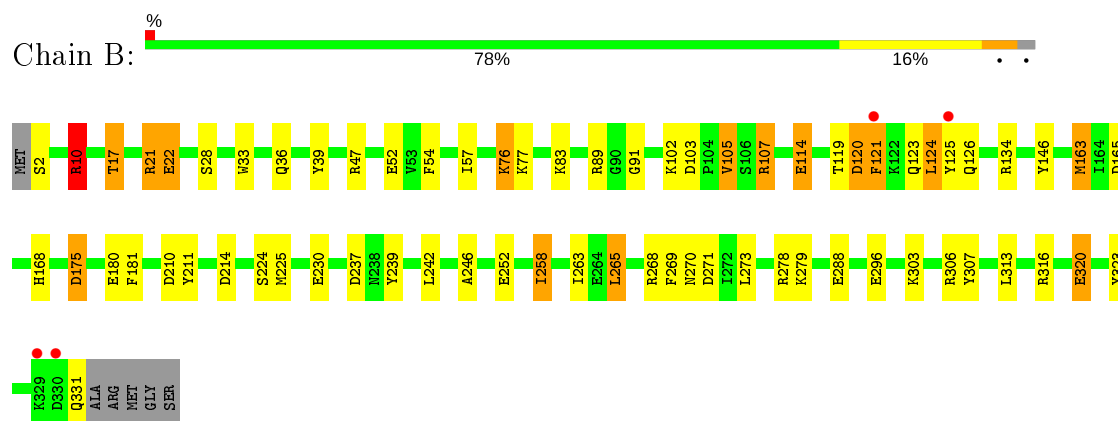
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	128.01Å 128.01Å 124.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.32 – 2.20 73.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	84.0 (73.32-2.20) 84.0 (73.23-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.194 , 0.243 0.202 , 0.247	Depositor DCC
$R_{free}$ test set	2294 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-l,-k 0.011 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5958	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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 24.18 % 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 4.0316e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 7PE, EMO, PEG, EDO, SO4

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	1.11	10/2891 (0.3%)	1.09	17/3910 (0.4%)
1	B	1.11	10/2863 (0.3%)	1.05	15/3872 (0.4%)
All	All	1.11	20/5754 (0.3%)	1.07	32/7782 (0.4%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	GLU	CB-CG	7.61	1.66	1.52
1	B	114	GLU	CB-CG	7.48	1.66	1.52
1	A	39	TYR	CE1-CZ	-7.28	1.29	1.38
1	B	39	TYR	CE1-CZ	-7.16	1.29	1.38
1	B	211	TYR	CG-CD2	-6.40	1.30	1.39
1	A	39	TYR	CE2-CZ	-6.30	1.30	1.38
1	A	26	TYR	CE2-CZ	-6.20	1.30	1.38
1	A	39	TYR	CG-CD1	-5.91	1.31	1.39
1	B	211	TYR	CE1-CZ	-5.89	1.30	1.38
1	B	211	TYR	CE2-CZ	-5.88	1.30	1.38
1	B	39	TYR	CE2-CZ	-5.87	1.30	1.38
1	A	26	TYR	CE1-CZ	-5.77	1.31	1.38
1	A	89	ARG	CZ-NH1	-5.51	1.25	1.33
1	B	54	PHE	CE1-CZ	-5.47	1.26	1.37
1	B	181	PHE	CE2-CZ	-5.34	1.27	1.37
1	A	211	TYR	CE2-CZ	-5.23	1.31	1.38
1	B	320	GLU	CB-CG	-5.18	1.42	1.52
1	A	39	TYR	CG-CD2	-5.10	1.32	1.39
1	A	10	ARG	CZ-NH1	-5.10	1.26	1.33
1	B	76	LYS	CD-CE	5.07	1.64	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	NE-CZ-NH2	13.01	126.81	120.30
1	A	280	ARG	NE-CZ-NH1	-12.16	114.22	120.30
1	A	278	ARG	NE-CZ-NH2	-11.03	114.78	120.30
1	A	10	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	B	278	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	A	316	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	180	GLU	OE1-CD-OE2	-8.01	113.69	123.30
1	A	278	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	210	ASP	CB-CG-OD1	7.71	125.23	118.30
1	A	312	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	B	10	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	280	ARG	CD-NE-CZ	6.83	133.16	123.60
1	B	180	GLU	OE1-CD-OE2	-6.55	115.44	123.30
1	B	89	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	210	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	320	GLU	CB-CA-C	-5.88	98.63	110.40
1	A	8	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	320	GLU	CB-CA-C	-5.72	98.97	110.40
1	B	316	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	B	124	LEU	CA-CB-CG	5.64	128.26	115.30
1	B	163	MET	CG-SD-CE	5.60	109.16	100.20
1	B	224	SER	CB-CA-C	-5.60	99.46	110.10
1	A	306	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	153	MET	CG-SD-CE	-5.34	91.66	100.20
1	A	280	ARG	CG-CD-NE	-5.33	100.61	111.80
1	B	306	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	316	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	A	10	ARG	CD-NE-CZ	5.21	130.90	123.60
1	B	214	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	195	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	76	LYS	CD-CE-NZ	5.02	123.24	111.70
1	B	21	ARG	CB-CG-CD	-5.00	98.59	111.60

There are no chirality outliers.

There are no planarity outliers.

## 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	2812	0	2754	54	1
1	B	2788	0	2730	47	1
2	A	20	0	9	2	0
2	B	20	0	9	0	0
3	A	4	0	6	1	0
3	B	4	0	6	1	0
4	A	21	0	30	12	0
5	A	15	0	0	0	0
5	B	20	0	0	2	0
6	B	7	0	10	0	0
7	A	116	0	0	6	0
7	B	131	0	0	12	0
All	All	5958	0	5554	103	1

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 9.

All (103) 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:36:GLN:NE2	1:A:104:PRO:HD3	1.10	1.39
1:A:36:GLN:NE2	1:A:104:PRO:CD	2.03	1.21
1:A:36:GLN:HE22	1:A:104:PRO:CD	1.58	1.15
1:B:239:TYR:CD2	1:B:269:PHE:HE2	1.66	1.12
1:B:239:TYR:HD2	1:B:269:PHE:CE2	1.70	1.08
1:B:239:TYR:CD2	1:B:269:PHE:CE2	2.43	1.07
1:B:107:ARG:HG3	1:B:107:ARG:HH11	1.21	1.05
1:A:36:GLN:HE21	1:A:104:PRO:HD3	1.18	0.93
1:B:242:LEU:HD23	1:B:269:PHE:CE1	2.06	0.89
1:B:242:LEU:CD2	1:B:269:PHE:HE1	1.89	0.86
1:A:242:LEU:HD23	1:A:269:PHE:CE1	2.15	0.82
1:A:17:THR:HG22	7:A:342:HOH:O	1.82	0.79
1:B:107:ARG:NH1	5:B:341:SO4:O4	2.16	0.78
1:A:17:THR:HG21	7:A:414:HOH:O	1.83	0.78
1:A:25:ASP:HA	3:A:337:EDO:H22	1.65	0.76
1:B:17:THR:HG22	7:B:344:HOH:O	1.88	0.73
1:A:253:ASP:OD1	4:A:338:7PE:H62	1.89	0.73
1:B:103:ASP:OD1	1:B:105:VAL:HG12	1.88	0.73
1:A:240:ASP:O	1:A:244:ARG:HG2	1.89	0.72
1:A:120:ASP:OD2	1:A:122:LYS:HB2	1.90	0.72
1:A:280:ARG:HH11	4:A:338:7PE:H182	1.55	0.71
1:A:194:SER:HB3	7:A:416:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ASP:HB2	7:B:452:HOH:O	1.90	0.70
1:A:102:LYS:HE2	1:A:107:ARG:O	1.91	0.70
1:A:108:THR:HB	1:A:109:PRO:HD2	1.73	0.70
1:A:194:SER:CB	7:A:416:HOH:O	2.40	0.69
1:A:108:THR:HB	1:A:109:PRO:CD	2.25	0.67
1:A:268:ARG:HD2	7:A:415:HOH:O	1.96	0.66
1:A:36:GLN:HE22	1:A:104:PRO:HD3	0.83	0.66
1:B:239:TYR:CE2	1:B:269:PHE:HE2	2.12	0.63
1:A:78:ILE:HD13	1:A:109:PRO:HG2	1.82	0.62
1:A:278:ARG:H	4:A:338:7PE:C11	2.12	0.62
1:B:242:LEU:HD22	1:B:269:PHE:HE1	1.64	0.61
1:B:28:SER:OG	7:B:397:HOH:O	1.96	0.61
1:B:331:GLN:C	7:B:436:HOH:O	2.39	0.60
1:A:277:SER:HB2	4:A:338:7PE:H122	1.85	0.59
1:A:118:ASN:HB2	1:A:163:MET:CE	2.33	0.58
1:B:107:ARG:HD2	1:B:107:ARG:N	2.18	0.58
1:B:242:LEU:CD2	1:B:269:PHE:CE1	2.72	0.57
1:A:118:ASN:HD22	1:A:164:ILE:H	1.50	0.57
1:B:114:GLU:HG3	1:B:114:GLU:O	2.05	0.57
1:A:283:ARG:HD2	4:A:338:7PE:H211	1.86	0.56
1:B:107:ARG:CG	1:B:107:ARG:HH11	2.08	0.56
1:A:114:GLU:HG3	1:A:114:GLU:O	2.06	0.56
1:B:239:TYR:HD2	1:B:269:PHE:CD2	2.20	0.56
1:B:270:ASN:HB3	7:B:434:HOH:O	2.06	0.56
1:A:278:ARG:H	4:A:338:7PE:H112	1.70	0.54
1:B:239:TYR:CE2	1:B:269:PHE:CE2	2.92	0.53
1:A:36:GLN:HE22	1:A:104:PRO:CG	2.20	0.53
1:A:266:ASP:OD1	1:A:268:ARG:HB2	2.09	0.52
1:B:83:LYS:NZ	7:B:395:HOH:O	2.27	0.52
1:A:242:LEU:HD23	1:A:269:PHE:HE1	1.71	0.52
1:A:22:GLU:HG3	7:B:445:HOH:O	2.11	0.51
1:B:107:ARG:HG3	1:B:107:ARG:NH1	2.01	0.51
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.47	0.49
1:A:61:ASN:OD1	1:A:63:GLU:HG2	2.12	0.49
1:B:134:ARG:HG2	1:B:323:TYR:CZ	2.46	0.49
1:A:118:ASN:HB2	1:A:163:MET:HE1	1.92	0.49
1:A:278:ARG:HB3	4:A:338:7PE:H112	1.93	0.49
1:A:165:ASP:OD2	1:A:168:HIS:HD2	1.96	0.48
1:B:279:LYS:HZ1	3:B:338:EDO:H22	1.78	0.48
1:A:118:ASN:HB2	1:A:163:MET:HE2	1.95	0.48
1:A:242:LEU:HD23	1:A:269:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:TYR:CD2	1:B:269:PHE:CD2	2.99	0.48
1:B:121:PHE:CZ	1:B:225:MET:SD	3.07	0.48
1:A:283:ARG:HH11	4:A:338:7PE:H211	1.78	0.47
1:B:258:ILE:HD13	1:B:263:ILE:O	2.14	0.47
1:B:165:ASP:OD2	1:B:168:HIS:HD2	1.97	0.47
1:A:36:GLN:HE21	1:A:104:PRO:CD	2.01	0.47
4:A:338:7PE:H51	4:A:338:7PE:H22	1.52	0.47
1:A:91:GLY:HA3	1:A:146:TYR:CE2	2.50	0.47
1:A:278:ARG:HB2	4:A:338:7PE:H82	1.97	0.46
1:B:57:ILE:HD13	7:B:463:HOH:O	2.16	0.46
1:B:10:ARG:HG2	7:B:433:HOH:O	2.16	0.45
1:B:242:LEU:HD23	1:B:269:PHE:CD1	2.48	0.45
1:B:246:ALA:HA	1:B:307:TYR:OH	2.17	0.45
1:A:126:GLN:HA	1:A:126:GLN:HE21	1.82	0.44
1:B:303:LYS:HB3	1:B:313:LEU:HG	2.00	0.44
1:A:246:ALA:HA	1:A:307:TYR:OH	2.17	0.44
1:B:252:GLU:HG3	7:B:438:HOH:O	2.17	0.44
1:B:2:SER:OG	1:B:2:SER:O	2.31	0.44
1:B:52:GLU:HG3	7:B:387:HOH:O	2.17	0.43
1:A:269:PHE:HB3	1:A:273:LEU:HD22	1.99	0.43
2:A:400:EMO:O1	2:A:400:EMO:O19	2.31	0.43
1:B:175:ASP:OD2	7:B:458:HOH:O	2.21	0.43
1:A:174:ILE:HD12	2:A:400:EMO:C5	2.49	0.43
1:B:134:ARG:HD3	1:B:323:TYR:O	2.20	0.42
1:A:36:GLN:NE2	1:A:104:PRO:CG	2.77	0.42
1:B:237:ASP:OD1	1:B:239:TYR:HB2	2.20	0.42
1:A:279:LYS:HA	4:A:338:7PE:H202	2.01	0.42
1:A:258:ILE:HD13	1:A:263:ILE:O	2.19	0.42
1:B:107:ARG:NH1	5:B:341:SO4:S	2.93	0.42
1:B:22:GLU:O	1:B:83:LYS:HE2	2.20	0.42
1:A:61:ASN:CG	1:A:63:GLU:HG2	2.40	0.41
1:A:278:ARG:O	4:A:338:7PE:H151	2.19	0.41
1:B:270:ASN:HD22	1:B:270:ASN:N	2.18	0.41
1:B:91:GLY:HA3	1:B:146:TYR:CE2	2.56	0.41
1:B:33:TRP:CH2	1:B:102:LYS:HE3	2.56	0.41
1:A:299:ASP:OD2	1:A:303:LYS:HE2	2.21	0.41
1:A:63:GLU:OE1	7:A:436:HOH:O	2.21	0.41
1:B:265:LEU:HA	1:B:265:LEU:HD23	1.93	0.41
1:B:120:ASP:HA	1:B:163:MET:HA	2.02	0.40
1:A:239:TYR:CD1	1:A:269:PHE:CE2	3.10	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLU:OE2	1:B:296:GLU:OE2[6_555]	2.07	0.13

## 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	331/336 (98%)	322 (97%)	9 (3%)	0	100	100
1	B	328/336 (98%)	314 (96%)	14 (4%)	0	100	100
All	All	659/672 (98%)	636 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	307/308 (100%)	292 (95%)	15 (5%)	25	31
1	B	304/308 (99%)	279 (92%)	25 (8%)	11	11
All	All	611/616 (99%)	571 (94%)	40 (6%)	16	19

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

Mol	Chain	Res	Type
1	A	2	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	17	THR
1	A	21	ARG
1	A	32	GLU
1	A	36	GLN
1	A	77	LYS
1	A	102	LYS
1	A	180	GLU
1	A	186	GLN
1	A	258	ILE
1	A	262	ASN
1	A	265	LEU
1	A	268	ARG
1	A	273	LEU
1	A	320	GLU
1	B	10	ARG
1	B	17	THR
1	B	21	ARG
1	B	22	GLU
1	B	36	GLN
1	B	47	ARG
1	B	76	LYS
1	B	77	LYS
1	B	105	VAL
1	B	107	ARG
1	B	119	THR
1	B	120	ASP
1	B	121	PHE
1	B	123	GLN
1	B	124	LEU
1	B	125	TYR
1	B	126	GLN
1	B	175	ASP
1	B	230	GLU
1	B	258	ILE
1	B	265	LEU
1	B	268	ARG
1	B	273	LEU
1	B	288	GLU
1	B	320	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	36	GLN
1	A	126	GLN
1	A	168	HIS
1	A	262	ASN
1	A	270	ASN
1	A	290	GLN
1	A	331	GLN
1	B	118	ASN
1	B	126	GLN
1	B	168	HIS
1	B	270	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

13 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$
2	EMO	B	401	-	22,22,22	1.74	7 (31%)	34,34,34	1.13	3 (8%)
2	EMO	A	400	-	22,22,22	1.85	6 (27%)	34,34,34	1.31	4 (11%)
5	SO4	A	339	-	4,4,4	0.19	0	6,6,6	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	B	339	-	4,4,4	0.32	0	6,6,6	1.02	1 (16%)
3	EDO	A	337	-	3,3,3	0.39	0	2,2,2	0.42	0
5	SO4	A	341	-	4,4,4	0.20	0	6,6,6	0.26	0
6	PEG	B	337	-	6,6,6	0.64	0	5,5,5	0.80	0
5	SO4	B	341	-	4,4,4	0.25	0	6,6,6	0.42	0
5	SO4	B	342	-	4,4,4	0.29	0	6,6,6	0.62	0
3	EDO	B	338	-	3,3,3	0.52	0	2,2,2	0.42	0
5	SO4	A	340	-	4,4,4	0.25	0	6,6,6	0.72	0
5	SO4	B	340	-	4,4,4	0.38	0	6,6,6	0.51	0
4	7PE	A	338	-	20,20,20	0.61	0	19,19,19	0.65	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	EMO	B	401	-	-	-	0/3/3/3
2	EMO	A	400	-	-	-	0/3/3/3
3	EDO	A	337	-	-	1/1/1/1	-
6	PEG	B	337	-	-	3/4/4/4	-
3	EDO	B	338	-	-	1/1/1/1	-
4	7PE	A	338	-	-	10/18/18/18	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	EMO	C7-C6	-3.78	1.40	1.48
2	A	400	EMO	C8-C9	3.29	1.44	1.39
2	B	401	EMO	C7-C6	-3.25	1.41	1.48
2	B	401	EMO	C5-C6	-3.23	1.41	1.48
2	A	400	EMO	O19-C19	2.81	1.27	1.22
2	A	400	EMO	C5-C6	-2.72	1.42	1.48
2	B	401	EMO	O19-C19	2.68	1.27	1.22
2	B	401	EMO	C20-C19	-2.51	1.41	1.47
2	A	400	EMO	O6-C6	2.47	1.27	1.22
2	B	401	EMO	C18-C19	-2.44	1.41	1.47
2	B	401	EMO	O6-C6	2.44	1.27	1.22
2	A	400	EMO	C20-C19	-2.26	1.42	1.47
2	B	401	EMO	C8-C9	2.06	1.42	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	400	EMO	C5-C20-C1	2.94	121.14	118.41
2	A	400	EMO	O19-C19-C20	-2.90	116.73	121.43
2	B	401	EMO	C5-C20-C1	2.76	120.98	118.41
2	A	400	EMO	C1-C2-C3	-2.32	117.60	119.70
2	B	401	EMO	C10-C9-C16	-2.20	117.68	120.94
2	B	401	EMO	O19-C19-C20	-2.15	117.95	121.43
2	A	400	EMO	C4-C5-C20	-2.09	117.56	120.34
5	B	339	SO4	O4-S-O1	2.03	119.92	109.31

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	338	7PE	C17-C18-O19-C20
4	A	338	7PE	C2-C3-O4-C5
4	A	338	7PE	O4-C5-C6-O7
4	A	338	7PE	O10-C11-C12-O13
6	B	337	PEG	O2-C3-C4-O4
4	A	338	7PE	O13-C14-C15-O16
6	B	337	PEG	O1-C1-C2-O2
4	A	338	7PE	C18-C17-O16-C15
4	A	338	7PE	O16-C17-C18-O19
4	A	338	7PE	O7-C8-C9-O10
4	A	338	7PE	C6-C5-O4-C3
6	B	337	PEG	C4-C3-O2-C2
4	A	338	7PE	C12-C11-O10-C9
3	A	337	EDO	O1-C1-C2-O2
3	B	338	EDO	O1-C1-C2-O2

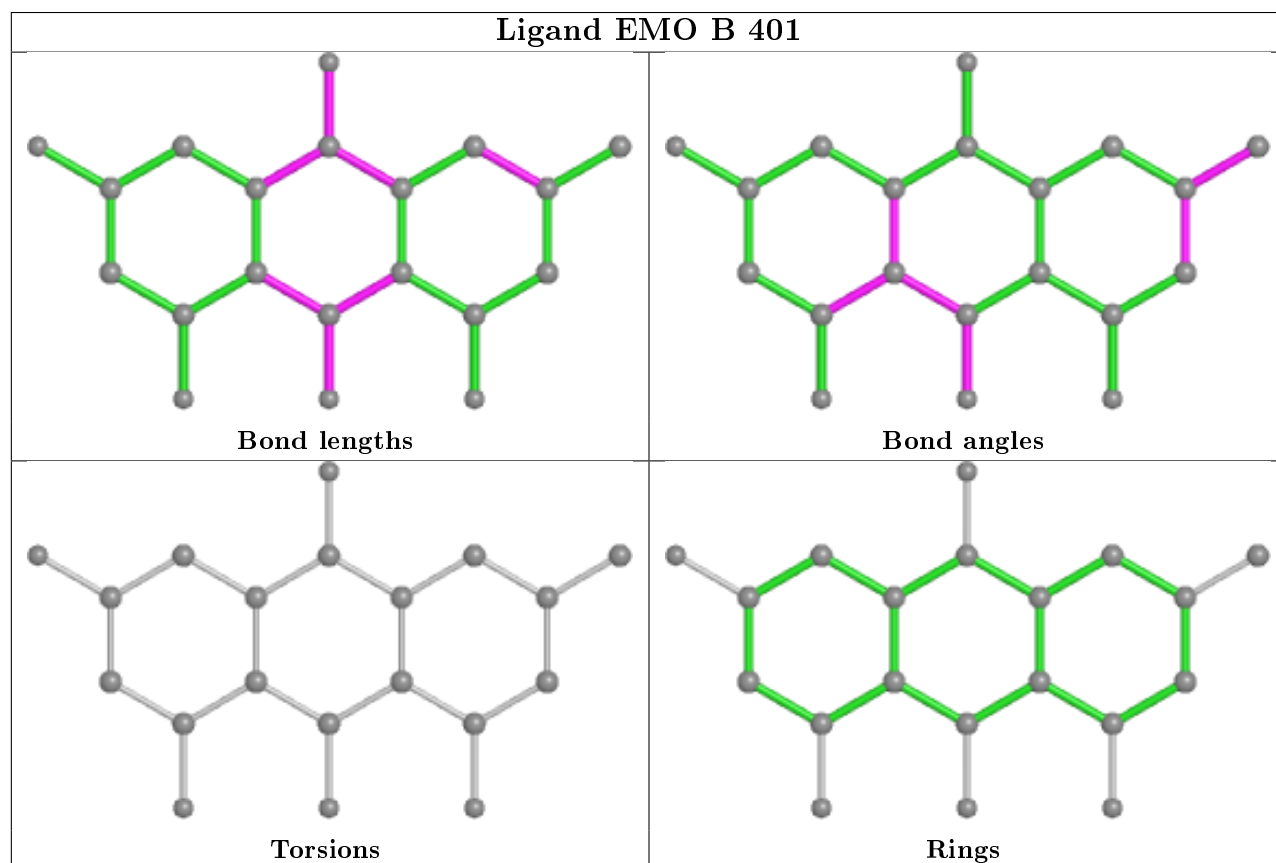
There are no ring outliers.

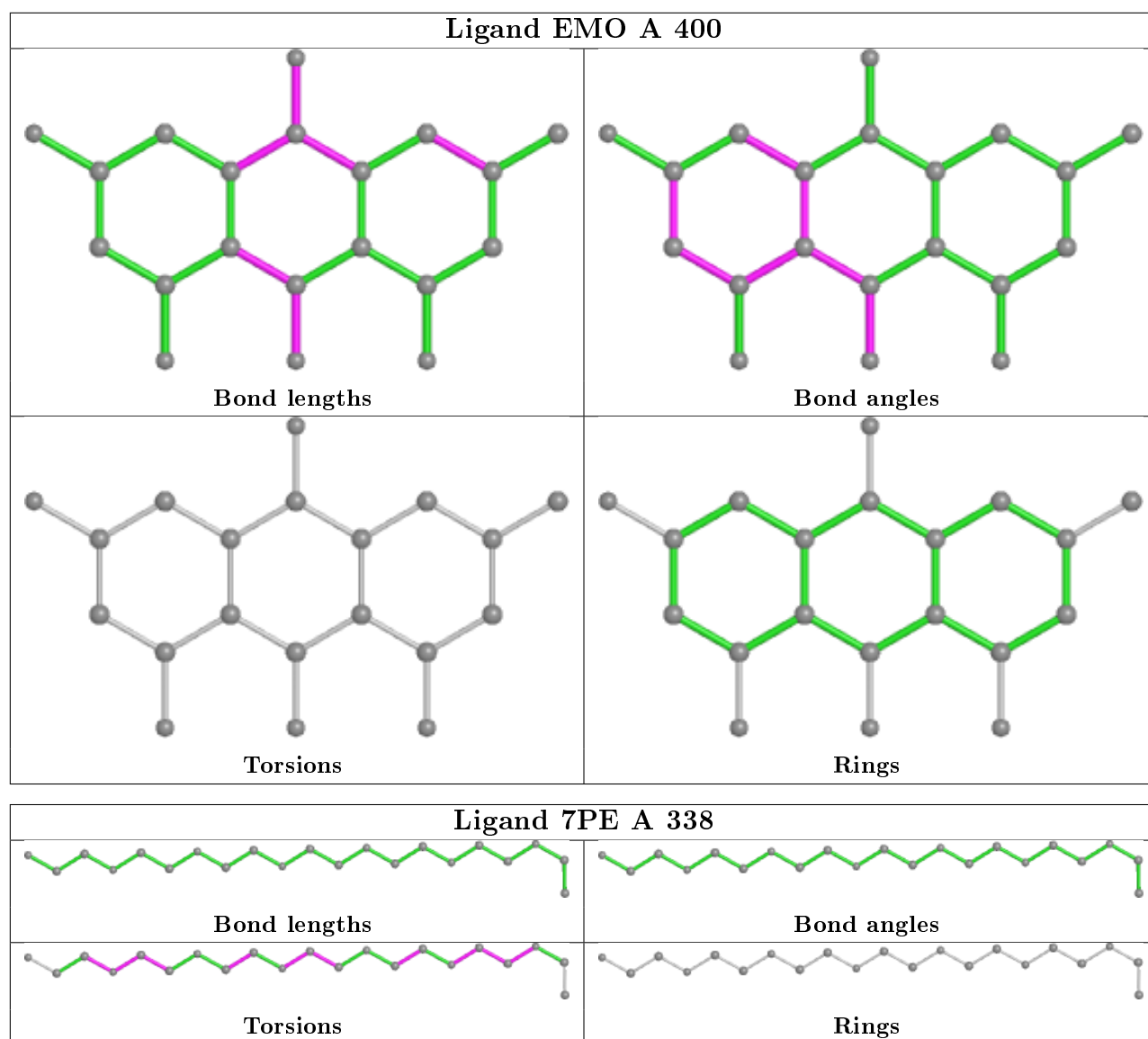
5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	EMO	2	0
3	A	337	EDO	1	0
5	B	341	SO4	2	0
3	B	338	EDO	1	0
4	A	338	7PE	12	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	330/336 (98%)	-0.27	1 (0%) 94 93	18, 31, 55, 69	0
1	B	330/336 (98%)	-0.24	4 (1%) 79 77	18, 31, 57, 82	0
All	All	660/672 (98%)	-0.25	5 (0%) 86 85	18, 31, 56, 82	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	PHE	7.4
1	B	125	TYR	3.3
1	A	2	SER	3.1
1	B	329	LYS	2.7
1	B	330	ASP	2.2

### 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](#)

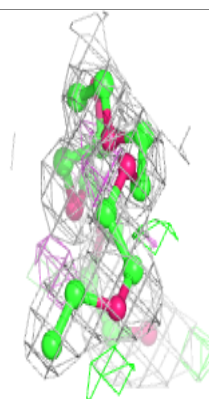
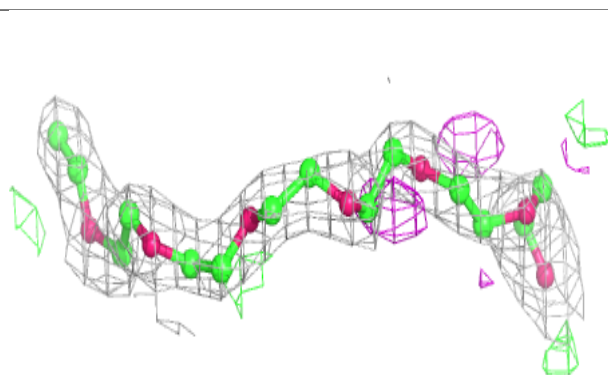
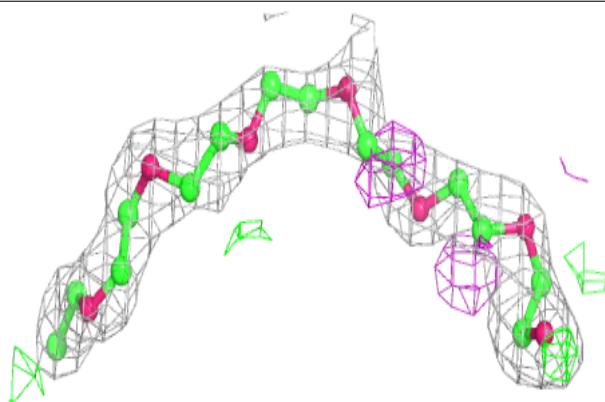
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PEG	B	337	7/7	0.86	0.18	45,49,55,59	0
3	EDO	B	338	4/4	0.88	0.14	48,51,51,52	0
4	7PE	A	338	21/21	0.88	0.25	32,48,54,56	0
5	SO4	A	341	5/5	0.91	0.13	96,96,97,98	0
2	EMO	A	400	20/20	0.92	0.13	23,28,35,36	0
5	SO4	A	339	5/5	0.93	0.19	72,73,75,77	0
2	EMO	B	401	20/20	0.94	0.09	28,34,39,39	0
5	SO4	B	342	5/5	0.94	0.14	74,75,76,77	0
5	SO4	A	340	5/5	0.96	0.14	53,54,55,55	0
5	SO4	B	340	5/5	0.97	0.14	44,47,50,51	0
5	SO4	B	341	5/5	0.98	0.11	53,54,56,57	0
5	SO4	B	339	5/5	0.98	0.12	40,43,46,46	0
3	EDO	A	337	4/4	0.98	0.17	30,34,39,41	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.

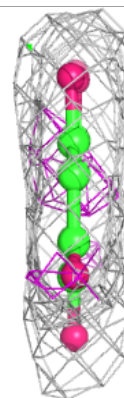
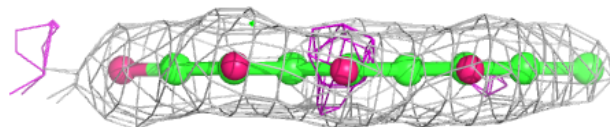
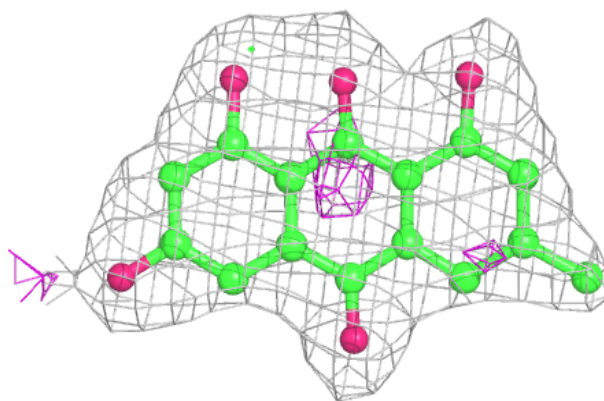
**Electron density around 7PE A 338:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

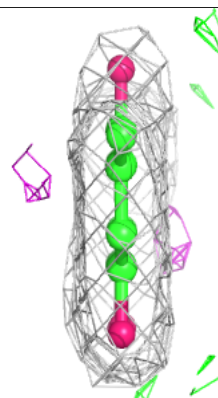
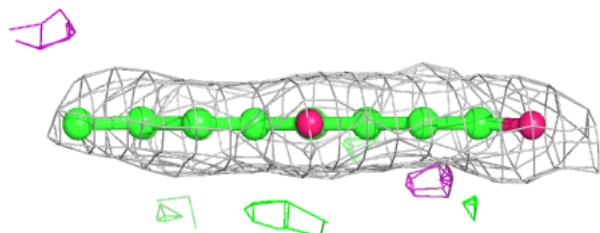
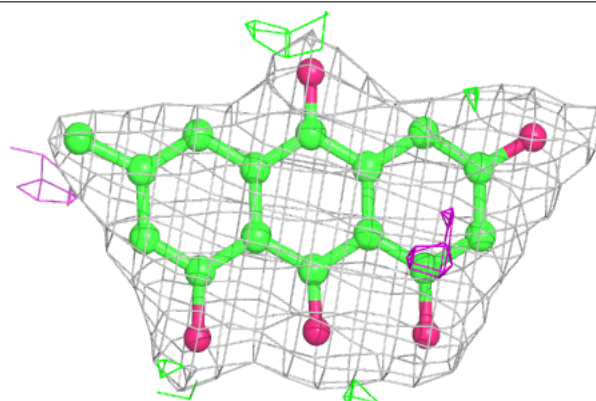


**Electron density around EMO A 400:**

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

**Electron density around EMO B 401:**

$2mF_o-DF_c$  (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.