



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:56 PM UTC

PDB ID : 7PI4 / pdb_00007pi4
Title : FAK Protac GSK215 in complex with FAK and pVHL:ElonginC:ElonginB
Authors : Chung, C.
Deposited on : 2021-08-19
Resolution : 2.24 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

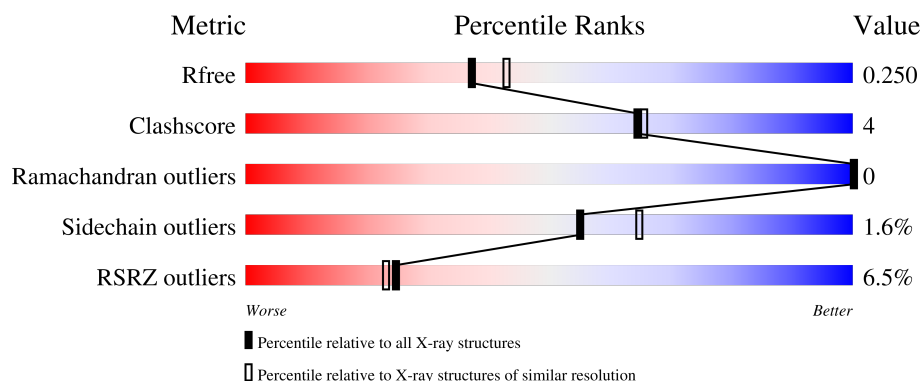
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	AAA	155	5% 89% 11%
2	BBB	105	2% 98% .
3	CCC	96	5% 85% 6% 7%
4	DDD	273	9% 85% 11% ..

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5240 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 von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	155	Total	C	N	O	S	0	1	0
			1276	806	238	228	4			

- Molecule 2 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	105	Total	C	N	O	S	0	0	0
			829	525	139	160	5			

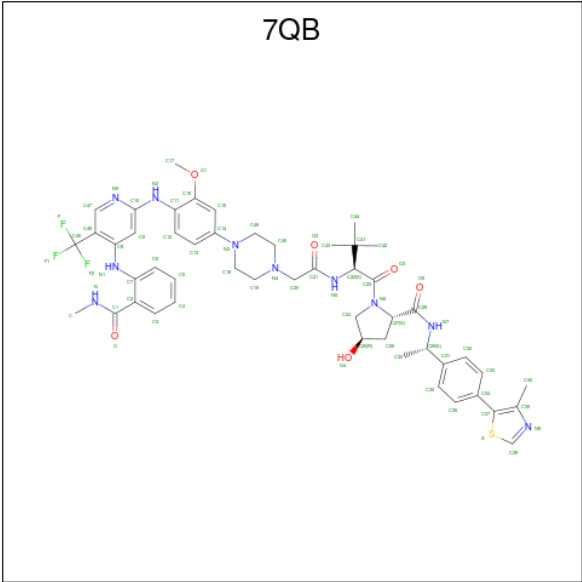
- Molecule 3 is a protein called Isoform 2 of Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	89	Total	C	N	O	S	0	0	0
			702	452	113	131	6			

- Molecule 4 is a protein called Focal adhesion kinase 1.

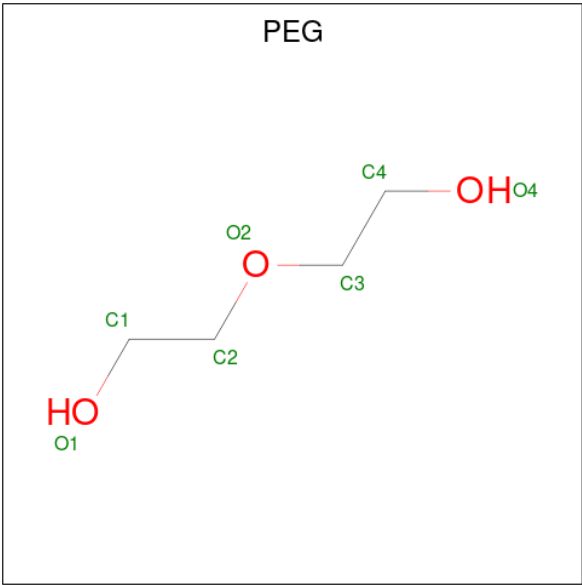
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	264	Total	C	N	O	S	0	0	0
			2128	1358	368	384	18			

- Molecule 5 is (2S,4R)-4-hydroxy-1-((S)-2-(2-(4-(3-methoxy-4-((4-((2-(methylcarbamoyl)phenyl)amino)-5-(trifluoromethyl)pyridin-2-yl)amino)phenyl)piperazin-1-yl)acetamido)-3,3-dimethylbutanoyl)-N-((S)-1-(4-(4-methylthiazol-5-yl)phenyl)ethyl)pyrrolidine-2-carboxamide (CCD ID: 7QB) (formula: C₅₀H₅₉F₃N₁₀O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	AAA	1	Total	C	F	N	O	S	0	0
			70	50	3	10	6	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



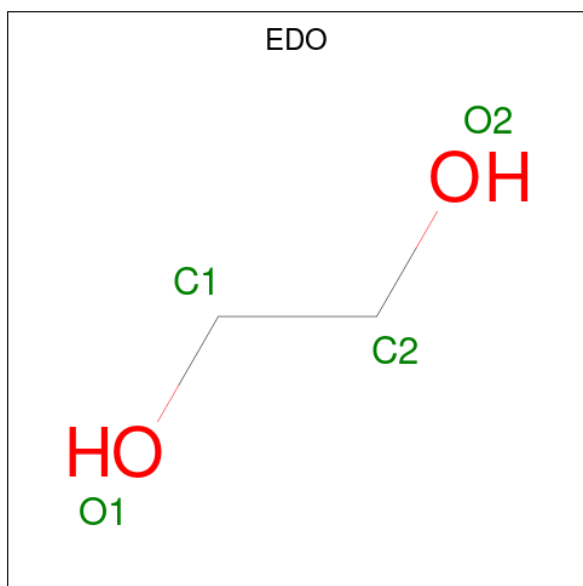
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	BBB	1	Total	C	O	0	0
			4	2	2		
7	BBB	1	Total	C	O	0	0
			4	2	2		
7	CCC	1	Total	C	O	0	0
			4	2	2		
7	CCC	1	Total	C	O	0	0
			4	2	2		
7	CCC	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	1	Total	Ca	0	0
			1	1		

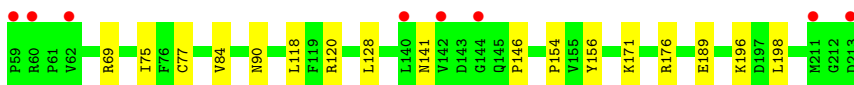
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	46	Total	O	0	0
			46	46		
9	BBB	37	Total	O	0	0
			37	37		
9	CCC	24	Total	O	0	0
			24	24		
9	DDD	43	Total	O	0	0
			43	43		

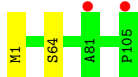
3 Residue-property plots [i](#)

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.

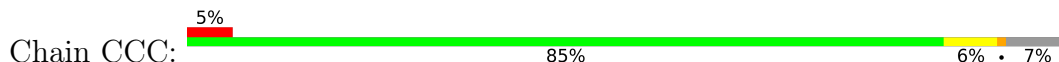
- Molecule 1: von Hippel-Lindau disease tumor suppressor



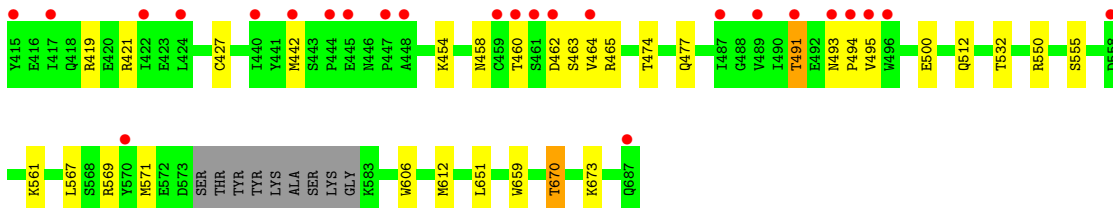
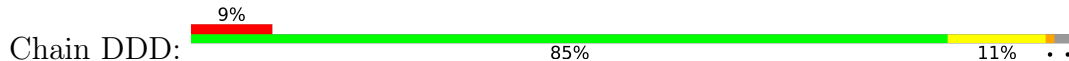
- Molecule 2: Elongin-B



- Molecule 3: Isoform 2 of Elongin-C



- Molecule 4: Focal adhesion kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.55Å 77.26Å 175.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.38 – 2.24 56.38 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.38-2.24) 99.9 (56.38-2.24)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.195 , 0.251 0.199 , 0.250	Depositor DCC
R_{free} test set	1963 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5240	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, CA, 7QB

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	AAA	0.96	0/1309	1.31	0/1783
2	BBB	0.94	0/846	1.25	0/1144
3	CCC	1.01	0/717	1.36	0/967
4	DDD	1.01	0/2175	1.42	0/2939
All	All	0.99	0/5047	1.36	0/6833

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	1276	0	1273	13	0
2	BBB	829	0	831	1	0
3	CCC	702	0	701	4	0
4	DDD	2128	0	2137	23	0
5	AAA	70	0	0	0	0
6	AAA	7	0	10	2	0
6	DDD	21	0	30	0	0
7	AAA	20	0	30	3	0
7	BBB	8	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	CCC	12	0	18	2	0
7	DDD	16	0	24	0	0
8	AAA	1	0	0	0	0
9	AAA	46	0	0	1	0
9	BBB	37	0	0	0	0
9	CCC	24	0	0	0	0
9	DDD	43	0	0	2	0
All	All	5240	0	5066	40	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 4.

All (40) 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)
3:CCC:17:MET:N	7:CCC:201:EDO:HO1	1.56	1.04
4:DDD:612:MET:HE1	4:DDD:651:LEU:HD11	1.39	1.04
4:DDD:612:MET:CE	4:DDD:651:LEU:HD11	2.15	0.77
4:DDD:465:ARG:NH1	4:DDD:491:THR:O	2.30	0.65
4:DDD:458:ASN:HB2	4:DDD:464:VAL:HG11	1.80	0.62
4:DDD:612:MET:HE1	4:DDD:651:LEU:CD1	2.25	0.61
3:CCC:17:MET:N	7:CCC:201:EDO:O1	2.32	0.59
4:DDD:458:ASN:N	4:DDD:458:ASN:HD22	2.01	0.59
4:DDD:670:THR:CG2	9:DDD:841:HOH:O	2.51	0.59
3:CCC:90:ILE:HD12	3:CCC:91:PRO:O	2.03	0.58
4:DDD:454:LYS:HD2	4:DDD:567:LEU:HD11	1.87	0.55
4:DDD:419:ARG:NH2	4:DDD:494:PRO:O	2.43	0.52
6:AAA:302:PEG:H21	4:DDD:512:GLN:HG3	1.92	0.51
4:DDD:532:THR:HA	4:DDD:673:LYS:HD2	1.93	0.50
4:DDD:460:THR:HG21	4:DDD:463:SER:HB3	1.95	0.49
1:AAA:90:ASN:HD22	7:AAA:306:EDO:C1	2.25	0.48
1:AAA:196:LYS:HD2	9:AAA:404:HOH:O	2.14	0.48
1:AAA:75:ILE:HG22	1:AAA:77[A]:CYS:SG	2.53	0.48
4:DDD:569:ARG:O	4:DDD:571:MET:HG2	2.14	0.48
4:DDD:500:GLU:OE2	4:DDD:561:LYS:NZ	2.45	0.47
4:DDD:606:TRP:CE3	4:DDD:659:TRP:HA	2.49	0.47
2:BBB:1:MET:HG2	2:BBB:64:SER:HB2	1.96	0.47
1:AAA:141:ASN:HD21	1:AAA:146:PRO:HA	1.81	0.46
1:AAA:141:ASN:ND2	1:AAA:146:PRO:HA	2.32	0.45
1:AAA:171:LYS:HG3	7:AAA:303:EDO:H11	1.99	0.44
4:DDD:458:ASN:N	4:DDD:458:ASN:ND2	2.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CCC:45:MET:HE2	3:CCC:60:VAL:HG13	2.00	0.44
4:DDD:460:THR:HG21	4:DDD:463:SER:CB	2.49	0.43
1:AAA:154:PRO:HG2	1:AAA:156:TYR:CE1	2.55	0.42
1:AAA:69:ARG:NH2	4:DDD:427:CYS:SG	2.92	0.42
6:AAA:302:PEG:C2	4:DDD:512:GLN:HG3	2.49	0.42
4:DDD:474:THR:HA	4:DDD:477:GLN:HE21	1.85	0.41
1:AAA:84:VAL:HG22	1:AAA:128:LEU:CD1	2.51	0.41
1:AAA:176:ARG:HH12	1:AAA:189:GLU:CD	2.28	0.41
1:AAA:90:ASN:HD22	7:AAA:306:EDO:H11	1.86	0.41
4:DDD:670:THR:HG23	9:DDD:841:HOH:O	2.17	0.41
1:AAA:118:LEU:HD13	1:AAA:120:ARG:HD3	2.01	0.41
1:AAA:198:LEU:HD23	1:AAA:198:LEU:HA	1.92	0.41
4:DDD:550:ARG:O	4:DDD:550:ARG:HD3	2.21	0.41
4:DDD:421:ARG:HB3	4:DDD:442:MET:O	2.22	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	AAA	154/155 (99%)	150 (97%)	4 (3%)	0	100	100
2	BBB	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
3	CCC	85/96 (88%)	85 (100%)	0	0	100	100
4	DDD	260/273 (95%)	256 (98%)	4 (2%)	0	100	100
All	All	602/629 (96%)	587 (98%)	15 (2%)	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	AAA	145/144 (101%)	145 (100%)	0	100	100
2	BBB	93/93 (100%)	93 (100%)	0	100	100
3	CCC	79/85 (93%)	76 (96%)	3 (4%)	29	34
4	DDD	235/242 (97%)	229 (97%)	6 (3%)	40	48
All	All	552/564 (98%)	543 (98%)	9 (2%)	55	65

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CCC	58	ASN
3	CCC	90	ILE
3	CCC	101	LEU
4	DDD	462	ASP
4	DDD	491	THR
4	DDD	493	ASN
4	DDD	495	VAL
4	DDD	555	SER
4	DDD	670	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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
6	PEG	DDD	702	-	6,6,6	0.21	0	5,5,5	0.15	0
7	EDO	BBB	201	-	3,3,3	0.13	0	2,2,2	0.19	0
7	EDO	CCC	203	-	3,3,3	0.13	0	2,2,2	0.06	0
7	EDO	DDD	705	-	3,3,3	0.13	0	2,2,2	0.15	0
7	EDO	BBB	202	-	3,3,3	0.15	0	2,2,2	0.28	0
6	PEG	DDD	701	-	6,6,6	0.20	0	5,5,5	0.09	0
7	EDO	CCC	202	-	3,3,3	0.07	0	2,2,2	0.03	0
6	PEG	DDD	703	-	6,6,6	0.23	0	5,5,5	0.14	0
7	EDO	DDD	707	-	3,3,3	0.08	0	2,2,2	0.33	0
7	EDO	AAA	303	-	3,3,3	0.17	0	2,2,2	0.28	0
7	EDO	AAA	304	-	3,3,3	0.08	0	2,2,2	0.14	0
7	EDO	AAA	305	-	3,3,3	0.16	0	2,2,2	0.06	0
7	EDO	DDD	704	-	3,3,3	0.03	0	2,2,2	0.04	0
7	EDO	CCC	201	-	3,3,3	0.05	0	2,2,2	0.11	0
7	EDO	AAA	307	-	3,3,3	0.21	0	2,2,2	0.26	0
7	EDO	AAA	306	-	3,3,3	0.12	0	2,2,2	0.09	0
7	EDO	DDD	706	-	3,3,3	0.09	0	2,2,2	0.17	0
5	7QB	AAA	301	-	75,76,76	0.35	0	108,111,111	0.60	0
6	PEG	AAA	302	-	6,6,6	0.17	0	5,5,5	0.18	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
6	PEG	DDD	702	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	BBB	201	-	-	1/1/1/1	-
7	EDO	CCC	203	-	-	1/1/1/1	-
7	EDO	DDD	705	-	-	1/1/1/1	-
7	EDO	BBB	202	-	-	1/1/1/1	-
6	PEG	DDD	701	-	-	1/4/4/4	-
7	EDO	CCC	202	-	-	1/1/1/1	-
6	PEG	DDD	703	-	-	0/4/4/4	-
7	EDO	DDD	707	-	-	0/1/1/1	-
7	EDO	AAA	303	-	-	1/1/1/1	-
7	EDO	AAA	304	-	-	1/1/1/1	-
7	EDO	AAA	305	-	-	1/1/1/1	-
7	EDO	DDD	704	-	-	1/1/1/1	-
7	EDO	CCC	201	-	-	1/1/1/1	-
7	EDO	AAA	307	-	-	1/1/1/1	-
7	EDO	AAA	306	-	-	0/1/1/1	-
7	EDO	DDD	706	-	-	0/1/1/1	-
5	7QB	AAA	301	-	-	0/64/86/86	0/7/7/7
6	PEG	AAA	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

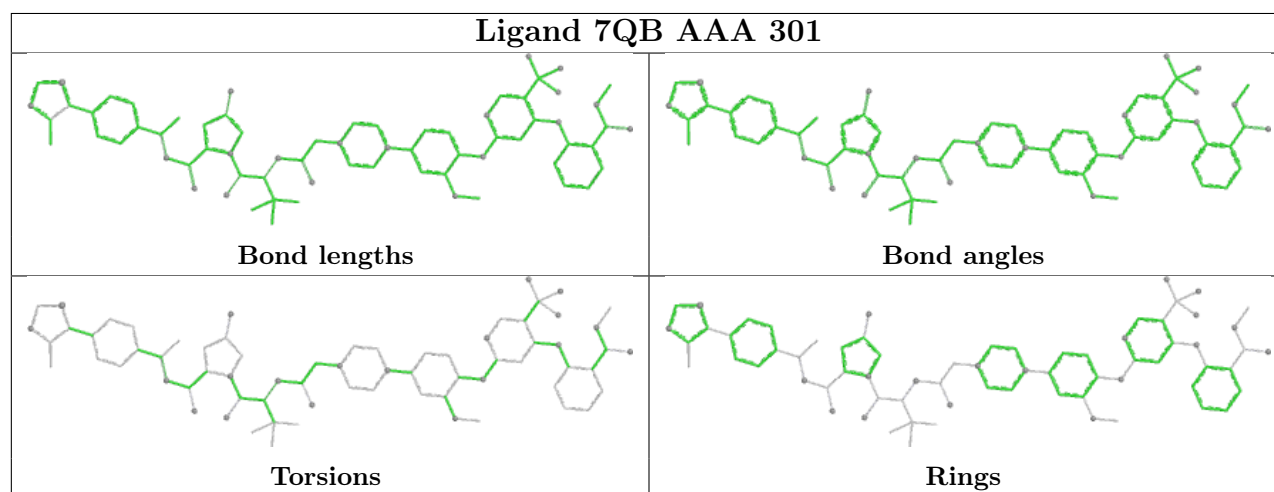
Mol	Chain	Res	Type	Atoms
6	AAA	302	PEG	O1-C1-C2-O2
6	DDD	702	PEG	O2-C3-C4-O4
7	BBB	202	EDO	O1-C1-C2-O2
7	DDD	705	EDO	O1-C1-C2-O2
6	DDD	701	PEG	O2-C3-C4-O4
7	AAA	303	EDO	O1-C1-C2-O2
7	AAA	304	EDO	O1-C1-C2-O2
7	CCC	203	EDO	O1-C1-C2-O2
6	DDD	702	PEG	O1-C1-C2-O2
7	AAA	305	EDO	O1-C1-C2-O2
7	AAA	307	EDO	O1-C1-C2-O2
7	BBB	201	EDO	O1-C1-C2-O2
7	CCC	202	EDO	O1-C1-C2-O2
7	DDD	704	EDO	O1-C1-C2-O2
7	CCC	201	EDO	O1-C1-C2-O2
6	AAA	302	PEG	O2-C3-C4-O4

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	AAA	303	EDO	1	0
7	CCC	201	EDO	2	0
7	AAA	306	EDO	2	0
6	AAA	302	PEG	2	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	AAA	155/155 (100%)	0.41	8 (5%)	33 31	25, 51, 88, 125	1 (0%)
2	BBB	105/105 (100%)	0.01	2 (1%)	66 68	35, 45, 66, 111	0
3	CCC	89/96 (92%)	0.14	5 (5%)	30 28	34, 44, 78, 138	0
4	DDD	264/273 (96%)	0.62	25 (9%)	14 12	37, 54, 110, 165	0
All	All	613/629 (97%)	0.39	40 (6%)	25 23	25, 50, 101, 165	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	59	PRO	6.4
4	DDD	415	TYR	5.7
2	BBB	105	PRO	5.4
1	AAA	140	LEU	4.9
4	DDD	495	VAL	4.8
4	DDD	442	MET	4.2
4	DDD	487	ILE	4.1
3	CCC	49	PRO	3.6
4	DDD	459	CYS	3.4
4	DDD	444	PRO	3.4
4	DDD	448	ALA	3.3
4	DDD	464	VAL	3.3
1	AAA	142	VAL	3.1
4	DDD	440	ILE	3.1
4	DDD	447	PRO	2.9
4	DDD	493	ASN	2.8
3	CCC	50	GLY	2.8
4	DDD	424	LEU	2.8
4	DDD	489	VAL	2.8
3	CCC	48	GLY	2.8
4	DDD	570	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	DDD	558	ASP	2.7
3	CCC	58	ASN	2.7
4	DDD	494	PRO	2.7
1	AAA	60	ARG	2.6
1	AAA	144	GLY	2.5
4	DDD	491	THR	2.5
4	DDD	461	SER	2.5
4	DDD	460	THR	2.4
4	DDD	445	GLU	2.4
1	AAA	62	VAL	2.3
4	DDD	687	GLN	2.3
3	CCC	88	THR	2.2
4	DDD	496	TRP	2.2
4	DDD	462	ASP	2.2
4	DDD	422	ILE	2.2
4	DDD	417	ILE	2.1
1	AAA	211	MET	2.0
2	BBB	81	ALA	2.0
1	AAA	213	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 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($\text{\AA}^2$)	Q<0.9
7	EDO	AAA	304	4/4	0.80	0.21	83,90,94,99	0
7	EDO	AAA	306	4/4	0.80	0.17	77,78,80,85	0
7	EDO	CCC	202	4/4	0.80	0.25	70,74,74,78	0
7	EDO	AAA	303	4/4	0.84	0.18	52,59,64,65	0

Continued on next page...

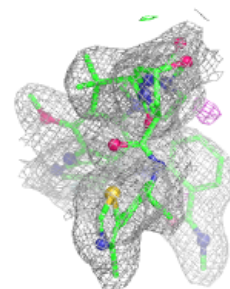
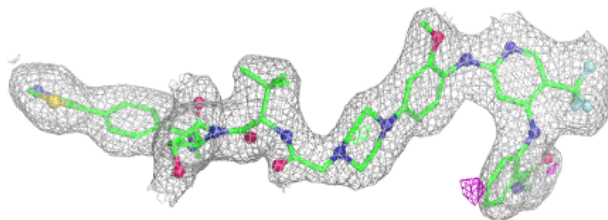
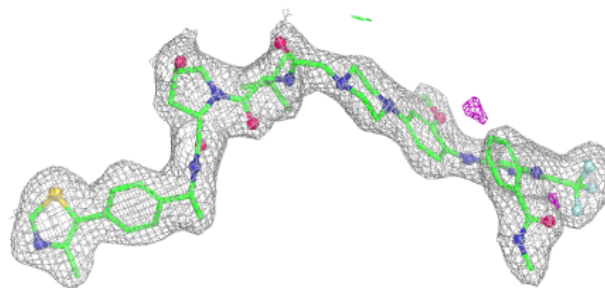
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	AAA	307	4/4	0.84	0.18	61,67,76,79	0
6	PEG	AAA	302	7/7	0.84	0.18	64,69,85,87	0
7	EDO	DDD	707	4/4	0.84	0.14	63,67,71,77	0
6	PEG	DDD	703	7/7	0.85	0.17	93,94,100,107	0
6	PEG	DDD	701	7/7	0.86	0.17	59,71,77,79	0
7	EDO	DDD	704	4/4	0.86	0.15	72,77,82,86	0
7	EDO	AAA	305	4/4	0.86	0.20	71,71,71,72	0
7	EDO	DDD	706	4/4	0.88	0.13	77,80,82,84	0
7	EDO	CCC	203	4/4	0.88	0.18	77,81,85,88	0
7	EDO	DDD	705	4/4	0.89	0.14	74,76,79,89	0
7	EDO	BBB	201	4/4	0.91	0.12	63,63,66,71	0
7	EDO	BBB	202	4/4	0.91	0.11	65,69,70,72	0
7	EDO	CCC	201	4/4	0.92	0.14	61,63,73,82	0
6	PEG	DDD	702	7/7	0.93	0.11	60,64,70,71	0
5	7QB	AAA	301	70/70	0.95	0.09	36,48,62,66	0
8	CA	AAA	308	1/1	0.99	0.06	47,47,47,47	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 7QB AAA 301:

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.