



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:11 PM UTC

PDB ID : 4C02 / pdb_00004c02
Title : Crystal structure of human ACVR1 (ALK2) in complex with FKBP12.6 and dorsomorphin
Authors : Williams, E.; Riesebo, E.; Vollmar, M.; Krojer, T.; Bradley, A.; Shrestha, L.; Kupinska, K.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Bullock, A.
Deposited on : 2013-07-31
Resolution : 2.17 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (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

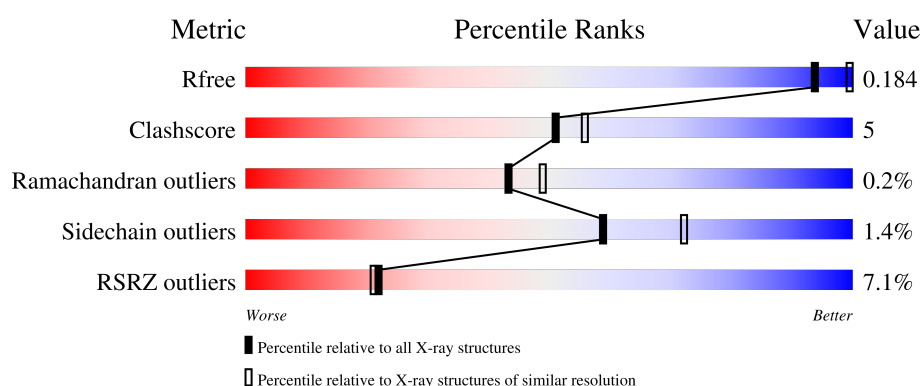
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	330	
2	B	108	

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	FLC	A	1500	-	X	-	-
3	FLC	A	1502	-	X	-	-
3	FLC	A	1504	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3756 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 ACTIVIN RECEPTOR TYPE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	313	2520	1618	428	459	15	0	11	0

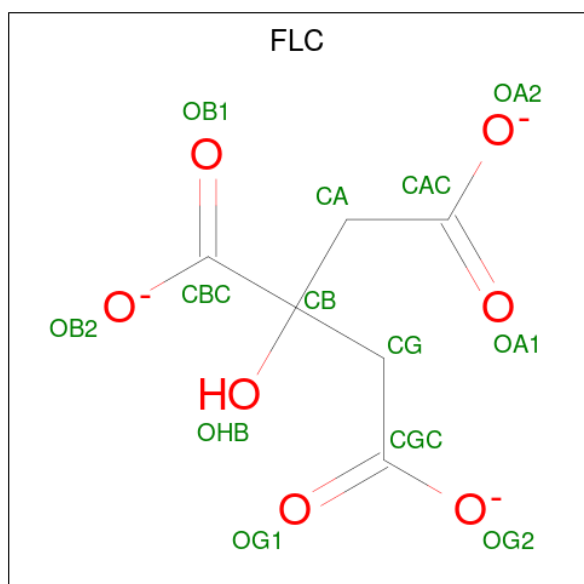
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	SER	-	expression tag	UNP Q04771
A	171	MET	-	expression tag	UNP Q04771

- Molecule 2 is a protein called PEPTIDYL-PROLYL CIS-TRANS ISOMERASE FKBP1B.

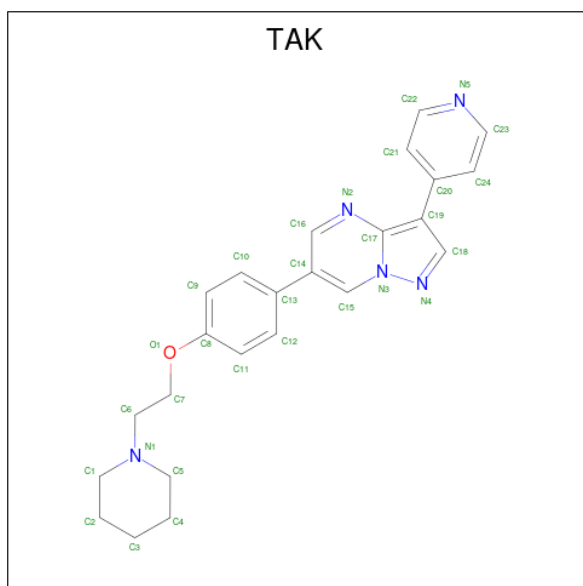
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	108	826	523	142	155	6	0	2	0

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7^-$).



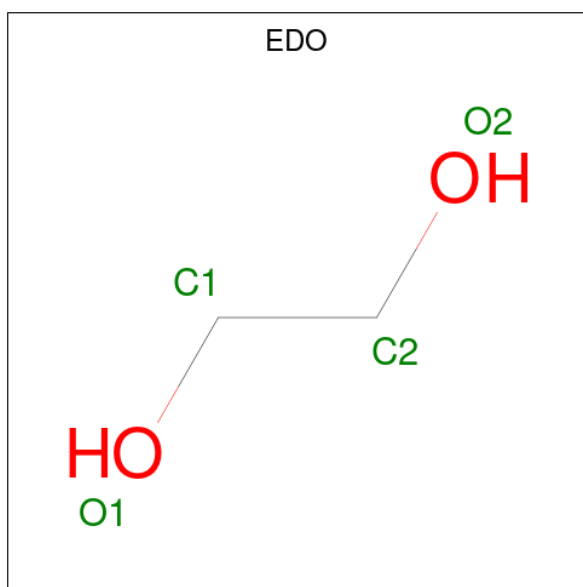
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 6-[4-(2-piperidin-1-ylethoxy)phenyl]-3-pyridin-4-ylpyrazolo[1,5-a]pyrimidine (CCD ID: TAK) (formula: C₂₄H₂₅N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	18	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

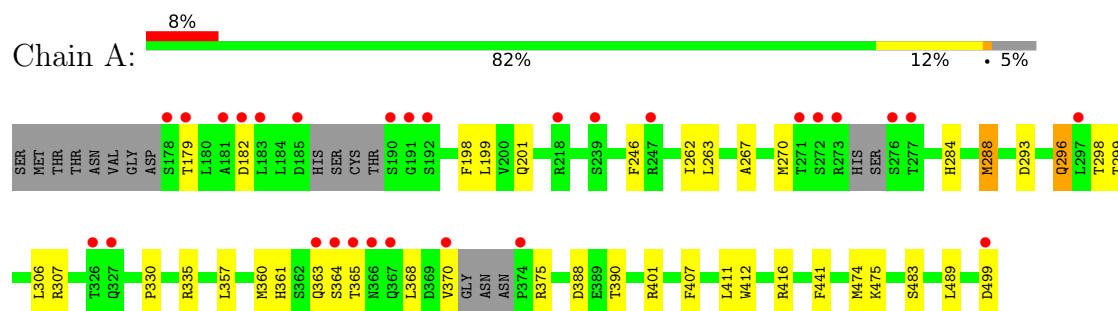
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	189	Total 189	O 189	0	0
6	B	42	Total 42	O 42	0	0

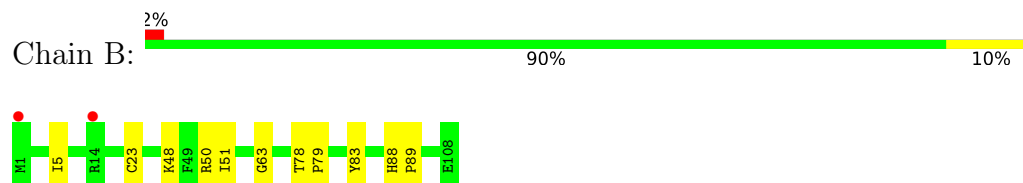
3 Residue-property plots

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: ACTIVIN RECEPTOR TYPE-1



• Molecule 2: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE FKBP1B



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	182.33Å 182.33Å 182.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.82 – 2.17 39.82 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.82-2.17) 99.8 (39.82-2.17)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.177 , 0.198 (Not available) , 0.184	Depositor DCC
R_{free} test set	2787 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3756	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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, TAK, FLC

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	0.78	0/2594	0.84	2/3520 (0.1%)
2	B	0.81	0/848	0.87	0/1144
All	All	0.79	0/3442	0.85	2/4664 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	GLN	N-CA-C	7.62	119.38	111.14
1	A	474	MET	CB-CA-C	-5.19	102.51	110.81

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	2520	0	2488	30	0
2	B	826	0	824	9	0
3	A	91	0	35	2	0
3	B	13	0	5	2	0
4	A	23	0	11	0	0
5	A	36	0	54	3	0
5	B	16	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	189	0	0	4	1
6	B	42	0	0	0	1
All	All	3756	0	3441	36	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 5.

All (36) 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:407[B]:PHE:CE1	1:A:411[B]:LEU:HD11	2.12	0.85
1:A:407[B]:PHE:HE1	1:A:411[B]:LEU:HD11	1.42	0.84
3:A:1502:FLC:OA1	3:A:1502:FLC:OB1	2.08	0.72
1:A:270:MET:HE1	3:B:1108:FLC:HG2	1.76	0.65
1:A:307:ARG:NH1	6:A:2060:HOH:O	2.31	0.62
1:A:293:ASP:OD2	6:A:2047:HOH:O	2.16	0.61
2:B:23[A]:CYS:SG	2:B:51:ILE:HD11	2.44	0.57
1:A:375:ARG:HD2	1:A:441:PHE:CE1	2.40	0.56
1:A:407[B]:PHE:CE1	1:A:411[B]:LEU:CD1	2.89	0.54
1:A:483[A]:SER:OG	6:A:2178:HOH:O	2.18	0.54
1:A:198[B]:PHE:CE1	2:B:88:HIS:CD2	2.96	0.53
1:A:284:HIS:HB2	5:A:1513:EDO:H11	1.90	0.52
1:A:198[B]:PHE:HE1	2:B:88:HIS:CD2	2.28	0.51
1:A:298:THR:HG22	1:A:299:THR:O	2.14	0.47
1:A:388[B]:ASP:OD1	1:A:390:THR:HG23	2.15	0.46
1:A:201:GLN:HB3	1:A:267:ALA:HB1	1.99	0.45
1:A:246:PHE:CD2	2:B:89:PRO:HG3	2.52	0.44
1:A:288:MET:HA	1:A:288:MET:HE2	2.00	0.44
1:A:361:HIS:ND1	6:A:2101:HOH:O	2.36	0.44
1:A:330:PRO:HG3	1:A:360:MET:HE3	2.01	0.43
1:A:489:LEU:HD23	3:A:1505:FLC:HA2	2.00	0.43
1:A:306:LEU:HD13	1:A:499:ASP:HA	2.01	0.43
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:HA	1.83	0.43
1:A:179:THR:HG23	1:A:182:ASP:H	1.84	0.43
1:A:401:ARG:HD2	5:A:1509:EDO:H21	2.01	0.42
1:A:270:MET:CE	3:B:1108:FLC:HG2	2.48	0.42
2:B:51:ILE:HG22	5:B:1112:EDO:H12	2.01	0.42
1:A:363:GLN:O	1:A:365:THR:N	2.50	0.42
1:A:475:LYS:HE2	5:A:1512:EDO:H12	2.02	0.41
2:B:78:THR:HB	2:B:79:PRO:HD2	2.02	0.41
1:A:335:ARG:HD3	1:A:357:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198[B]:PHE:CZ	2:B:83:TYR:CZ	3.09	0.40
2:B:5[A]:ILE:HD11	2:B:63:GLY:HA2	2.03	0.40
1:A:262:ILE:O	1:A:263:LEU:C	2.65	0.40
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2176:HOH:O	6:B:2037:HOH:O[6_445]	1.79	0.41

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	316/330 (96%)	307 (97%)	8 (2%)	1 (0%)	36	39
2	B	108/108 (100%)	105 (97%)	3 (3%)	0	100	100
All	All	424/438 (97%)	412 (97%)	11 (3%)	1 (0%)	43	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	SER

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	273/294 (93%)	269 (98%)	4 (2%)	57	70
2	B	88/89 (99%)	87 (99%)	1 (1%)	65	77
All	All	361/383 (94%)	356 (99%)	5 (1%)	59	72

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	LEU
1	A	288	MET
1	A	296	GLN
1	A	370	VAL
2	B	50	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	88	HIS

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](#)

22 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
3	FLC	B	1108	-	12,12,12	1.26	1 (8%)	17,17,17	1.84	4 (23%)
5	EDO	A	1513	-	3,3,3	0.41	0	2,2,2	0.32	0
5	EDO	B	1111	-	3,3,3	0.68	0	2,2,2	0.41	0
5	EDO	B	1109	-	3,3,3	0.56	0	2,2,2	0.24	0
5	EDO	A	1508	-	3,3,3	0.44	0	2,2,2	0.45	0
5	EDO	A	1511	-	3,3,3	0.50	0	2,2,2	0.46	0
5	EDO	A	1512	-	3,3,3	0.62	0	2,2,2	0.14	0
5	EDO	A	1514	-	3,3,3	0.51	0	2,2,2	0.31	0
3	FLC	A	1504	-	12,12,12	1.03	0	17,17,17	5.42	11 (64%)
3	FLC	A	1502	-	12,12,12	1.48	2 (16%)	17,17,17	5.42	9 (52%)
4	TAK	A	1507	-	25,26,34	1.82	4 (16%)	32,36,46	1.77	10 (31%)
5	EDO	B	1110	-	3,3,3	0.98	0	2,2,2	0.41	0
5	EDO	A	1510	-	3,3,3	0.60	0	2,2,2	0.18	0
5	EDO	B	1112	-	3,3,3	0.73	0	2,2,2	0.47	0
3	FLC	A	1506	-	12,12,12	1.27	0	17,17,17	1.96	4 (23%)
5	EDO	A	1509	-	3,3,3	0.51	0	2,2,2	0.51	0
3	FLC	A	1501	-	12,12,12	1.11	1 (8%)	17,17,17	1.27	2 (11%)
3	FLC	A	1503	-	12,12,12	1.45	1 (8%)	17,17,17	1.38	3 (17%)
3	FLC	A	1505	-	12,12,12	1.19	1 (8%)	17,17,17	1.01	1 (5%)
5	EDO	A	1515	-	3,3,3	0.46	0	2,2,2	0.17	0
5	EDO	A	1516	-	3,3,3	0.41	0	2,2,2	0.89	0
3	FLC	A	1500	-	12,12,12	2.76	3 (25%)	17,17,17	3.47	8 (47%)

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	FLC	B	1108	-	-	4/16/16/16	-
5	EDO	A	1513	-	-	1/1/1/1	-
5	EDO	B	1111	-	-	1/1/1/1	-
5	EDO	B	1109	-	-	1/1/1/1	-
5	EDO	A	1508	-	-	0/1/1/1	-
5	EDO	A	1511	-	-	0/1/1/1	-
5	EDO	A	1512	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1514	-	-	1/1/1/1	-
3	FLC	A	1504	-	-	10/16/16/16	-
3	FLC	A	1502	-	-	12/16/16/16	-
4	TAK	A	1507	-	-	0/10/10/22	0/4/4/5
5	EDO	B	1110	-	-	1/1/1/1	-
5	EDO	A	1510	-	-	0/1/1/1	-
5	EDO	B	1112	-	-	1/1/1/1	-
3	FLC	A	1506	-	-	11/16/16/16	-
5	EDO	A	1509	-	-	1/1/1/1	-
3	FLC	A	1501	-	-	6/16/16/16	-
3	FLC	A	1503	-	-	2/16/16/16	-
3	FLC	A	1505	-	-	3/16/16/16	-
5	EDO	A	1515	-	-	0/1/1/1	-
5	EDO	A	1516	-	-	1/1/1/1	-
3	FLC	A	1500	-	-	7/16/16/16	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1500	FLC	CB-CBC	-7.97	1.45	1.53
4	A	1507	TAK	C20-C19	-5.48	1.40	1.48
4	A	1507	TAK	O1-C8	3.62	1.44	1.37
4	A	1507	TAK	C17-N3	-3.39	1.31	1.38
3	A	1503	FLC	CB-CBC	-2.77	1.50	1.53
3	A	1502	FLC	CB-CBC	2.77	1.56	1.53
3	A	1500	FLC	CG-CB	2.59	1.57	1.54
4	A	1507	TAK	C18-N4	2.49	1.36	1.32
3	A	1500	FLC	OHB-CB	2.48	1.47	1.43
3	A	1505	FLC	OB1-CBC	2.26	1.29	1.22
3	A	1502	FLC	OA1-CAC	2.19	1.29	1.22
3	A	1501	FLC	OA2-CAC	-2.12	1.23	1.30
3	B	1108	FLC	CG-CB	2.04	1.56	1.54

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1504	FLC	OHB-CB-CBC	-15.02	87.66	108.96
3	A	1502	FLC	OHB-CB-CA	-13.28	79.10	109.38
3	A	1502	FLC	OHB-CB-CBC	-11.36	92.85	108.96
3	A	1500	FLC	OHB-CB-CBC	-9.88	94.94	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1504	FLC	OHB-CB-CG	-9.67	87.33	109.38
3	A	1504	FLC	OHB-CB-CA	-9.17	88.45	109.38
3	A	1502	FLC	OHB-CB-CG	-9.16	88.48	109.38
3	A	1500	FLC	OB1-CBC-CB	-5.89	110.68	122.09
3	A	1504	FLC	CG-CB-CA	5.73	124.01	109.31
3	A	1502	FLC	OB2-CBC-CB	5.64	123.95	113.14
3	A	1502	FLC	CA-CB-CBC	5.53	122.27	110.03
4	A	1507	TAK	C16-N2-C17	4.55	120.43	115.71
3	A	1500	FLC	OHB-CB-CG	4.54	119.74	109.38
3	A	1502	FLC	CG-CB-CA	4.47	120.79	109.31
3	A	1506	FLC	OHB-CB-CBC	-4.21	102.98	108.96
3	A	1506	FLC	OB2-CBC-CB	3.92	120.66	113.14
4	A	1507	TAK	C14-C16-N2	-3.90	121.84	125.38
3	A	1504	FLC	CA-CB-CBC	3.75	118.32	110.03
3	A	1506	FLC	OB1-CBC-CB	-3.54	115.23	122.09
3	A	1500	FLC	CG-CB-CBC	-3.33	102.67	110.03
3	A	1500	FLC	OB2-CBC-OB1	3.32	134.47	123.86
3	A	1504	FLC	CB-CG-CGC	-3.27	104.97	113.92
3	A	1504	FLC	CG-CB-CBC	3.26	117.24	110.03
3	B	1108	FLC	CB-CG-CGC	3.23	122.74	113.92
3	B	1108	FLC	OB2-CBC-CB	3.11	119.11	113.14
3	A	1501	FLC	CA-CB-CBC	-2.85	103.73	110.03
3	B	1108	FLC	CG-CB-CBC	2.83	116.29	110.03
4	A	1507	TAK	C21-C22-N5	-2.76	118.90	123.60
3	A	1503	FLC	OB1-CBC-CB	-2.74	116.79	122.09
3	A	1502	FLC	CG-CB-CBC	2.67	115.94	110.03
3	B	1108	FLC	OHB-CB-CBC	2.65	112.71	108.96
3	A	1500	FLC	OA2-CAC-CA	2.58	122.51	114.35
3	A	1500	FLC	OA1-CAC-CA	-2.51	115.84	122.95
3	A	1500	FLC	OG2-CGC-OG1	-2.47	116.98	123.33
4	A	1507	TAK	C18-N4-N3	2.36	106.12	103.81
3	A	1504	FLC	OB2-CBC-CB	2.36	117.66	113.14
4	A	1507	TAK	N3-C17-N2	-2.35	119.13	121.96
4	A	1507	TAK	C20-C19-C17	2.33	131.09	127.41
3	A	1506	FLC	OA2-CAC-CA	2.33	121.72	114.35
4	A	1507	TAK	C22-C21-C20	2.32	121.59	119.05
3	A	1504	FLC	OA1-CAC-CA	-2.30	116.43	122.95
3	A	1504	FLC	OA2-CAC-CA	2.27	121.53	114.35
4	A	1507	TAK	C19-C18-N4	-2.26	110.39	113.29
4	A	1507	TAK	C23-N5-C22	2.21	121.91	116.86
3	A	1503	FLC	OG2-CGC-CG	2.16	121.20	114.35
3	A	1503	FLC	OB2-CBC-CB	2.13	117.22	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1502	FLC	OG2-CGC-CG	2.12	121.06	114.35
3	A	1501	FLC	OB2-CBC-CB	2.12	117.20	113.14
3	A	1502	FLC	OB1-CBC-CB	-2.10	118.02	122.09
4	A	1507	TAK	C24-C20-C19	2.03	123.89	120.98
3	A	1504	FLC	OG1-CGC-CG	-2.01	117.25	122.95
3	A	1505	FLC	OA1-CAC-CA	-2.00	117.28	122.95

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1502	FLC	CA-CB-CBC-OB1
3	A	1502	FLC	CA-CB-CBC-OB2
3	A	1502	FLC	CG-CB-CBC-OB1
3	A	1502	FLC	CG-CB-CBC-OB2
3	A	1502	FLC	OHB-CB-CBC-OB1
3	A	1502	FLC	OHB-CB-CBC-OB2
3	A	1502	FLC	CBC-CB-CG-CGC
3	A	1502	FLC	OHB-CB-CG-CGC
3	A	1504	FLC	CAC-CA-CB-CG
3	A	1504	FLC	CG-CB-CBC-OB1
3	A	1504	FLC	CG-CB-CBC-OB2
3	A	1504	FLC	OHB-CB-CBC-OB1
3	A	1504	FLC	OHB-CB-CBC-OB2
3	A	1504	FLC	CA-CB-CG-CGC
3	A	1505	FLC	CBC-CB-CG-CGC
3	A	1505	FLC	OHB-CB-CG-CGC
3	A	1500	FLC	CA-CB-CG-CGC
3	A	1505	FLC	CA-CB-CG-CGC
3	B	1108	FLC	CA-CB-CG-CGC
3	B	1108	FLC	CBC-CB-CG-CGC
3	B	1108	FLC	OHB-CB-CG-CGC
3	A	1506	FLC	CAC-CA-CB-CG
3	A	1504	FLC	CA-CB-CBC-OB2
3	A	1506	FLC	CA-CB-CBC-OB2
3	A	1502	FLC	CAC-CA-CB-CBC
3	A	1504	FLC	CAC-CA-CB-OHB
3	A	1506	FLC	CAC-CA-CB-CBC
3	A	1506	FLC	OHB-CB-CG-CGC
5	A	1516	EDO	O1-C1-C2-O2
3	A	1502	FLC	CAC-CA-CB-CG
5	A	1512	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	1110	EDO	O1-C1-C2-O2
3	A	1503	FLC	CB-CG-CGC-OG1
3	A	1503	FLC	CB-CG-CGC-OG2
3	A	1501	FLC	CA-CB-CBC-OB2
3	A	1506	FLC	CA-CB-CG-CGC
3	A	1504	FLC	CA-CB-CBC-OB1
3	A	1506	FLC	CG-CB-CBC-OB2
3	A	1500	FLC	CBC-CB-CG-CGC
3	A	1506	FLC	CBC-CB-CG-CGC
3	A	1502	FLC	CB-CG-CGC-OG2
3	A	1506	FLC	OHB-CB-CBC-OB2
3	A	1501	FLC	CA-CB-CBC-OB1
3	A	1501	FLC	CG-CB-CBC-OB1
3	A	1501	FLC	CG-CB-CBC-OB2
3	A	1506	FLC	CA-CB-CBC-OB1
3	A	1506	FLC	CG-CB-CBC-OB1
5	A	1509	EDO	O1-C1-C2-O2
5	A	1513	EDO	O1-C1-C2-O2
5	A	1514	EDO	O1-C1-C2-O2
5	B	1109	EDO	O1-C1-C2-O2
5	B	1112	EDO	O1-C1-C2-O2
3	A	1502	FLC	CB-CG-CGC-OG1
3	A	1500	FLC	CG-CB-CBC-OB1
3	A	1500	FLC	CG-CB-CBC-OB2
3	A	1504	FLC	OHB-CB-CG-CGC
3	A	1500	FLC	OHB-CB-CG-CGC
3	A	1500	FLC	CB-CA-CAC-OA2
3	A	1501	FLC	OHB-CB-CBC-OB1
3	A	1501	FLC	OHB-CB-CBC-OB2
3	A	1506	FLC	OHB-CB-CBC-OB1
3	A	1500	FLC	CB-CA-CAC-OA1
5	B	1111	EDO	O1-C1-C2-O2
3	B	1108	FLC	CB-CA-CAC-OA1

There are no ring outliers.

7 monomers are involved in 8 short contacts:

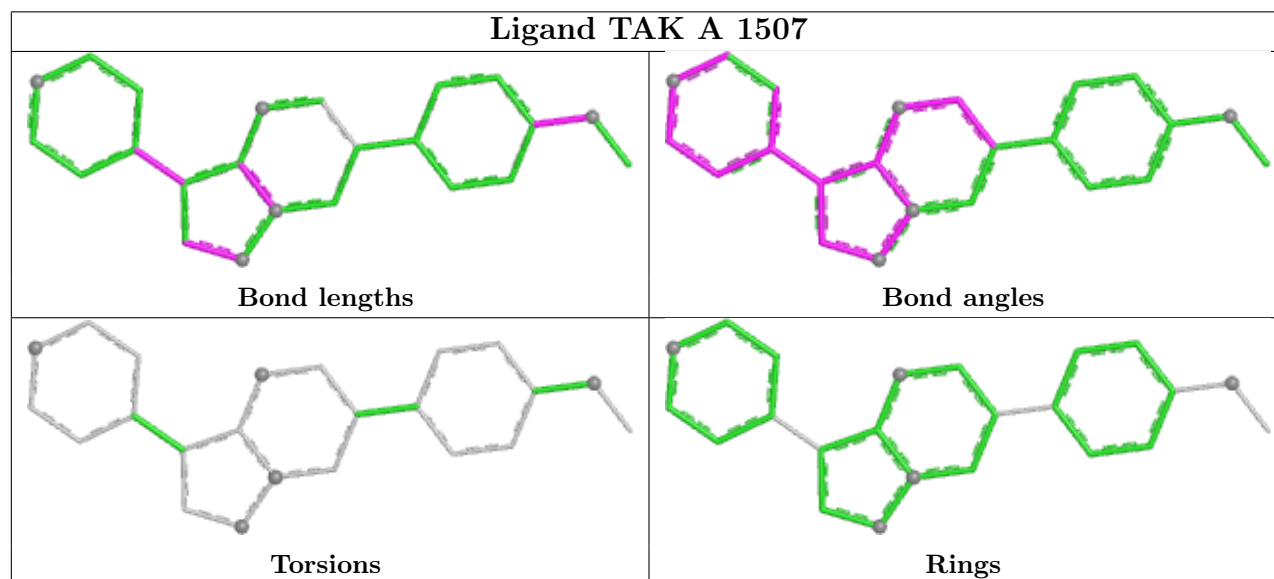
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1108	FLC	2	0
5	A	1513	EDO	1	0
5	A	1512	EDO	1	0
3	A	1502	FLC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1112	EDO	1	0
5	A	1509	EDO	1	0
3	A	1505	FLC	1	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	313/330 (94%)	0.10	28 (8%) 15 14	11, 30, 75, 113	11 (3%)
2	B	108/108 (100%)	-0.17	2 (1%) 66 65	18, 36, 57, 89	2 (1%)
All	All	421/438 (96%)	0.03	30 (7%) 22 21	11, 32, 72, 113	13 (3%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	SER	11.1
1	A	374	PRO	10.2
1	A	272	SER	9.2
1	A	370	VAL	9.2
1	A	276	SER	8.6
1	A	178	SER	8.3
1	A	273	ARG	7.3
1	A	191	GLY	6.6
1	A	364	SER	6.5
1	A	499	ASP	5.8
1	A	367	GLN	5.1
2	B	1	MET	4.8
1	A	297	LEU	4.2
1	A	277	THR	4.2
1	A	192	SER	3.7
1	A	185	ASP	3.6
1	A	271	THR	3.2
1	A	326	THR	3.2
1	A	365	THR	3.0
1	A	363	GLN	2.9
1	A	218	ARG	2.7
1	A	182	ASP	2.7
1	A	183	LEU	2.5
2	B	14	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	239	SER	2.4
1	A	179	THR	2.2
1	A	247	ARG	2.2
1	A	327	GLN	2.1
1	A	366	ASN	2.0
1	A	181	ALA	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.

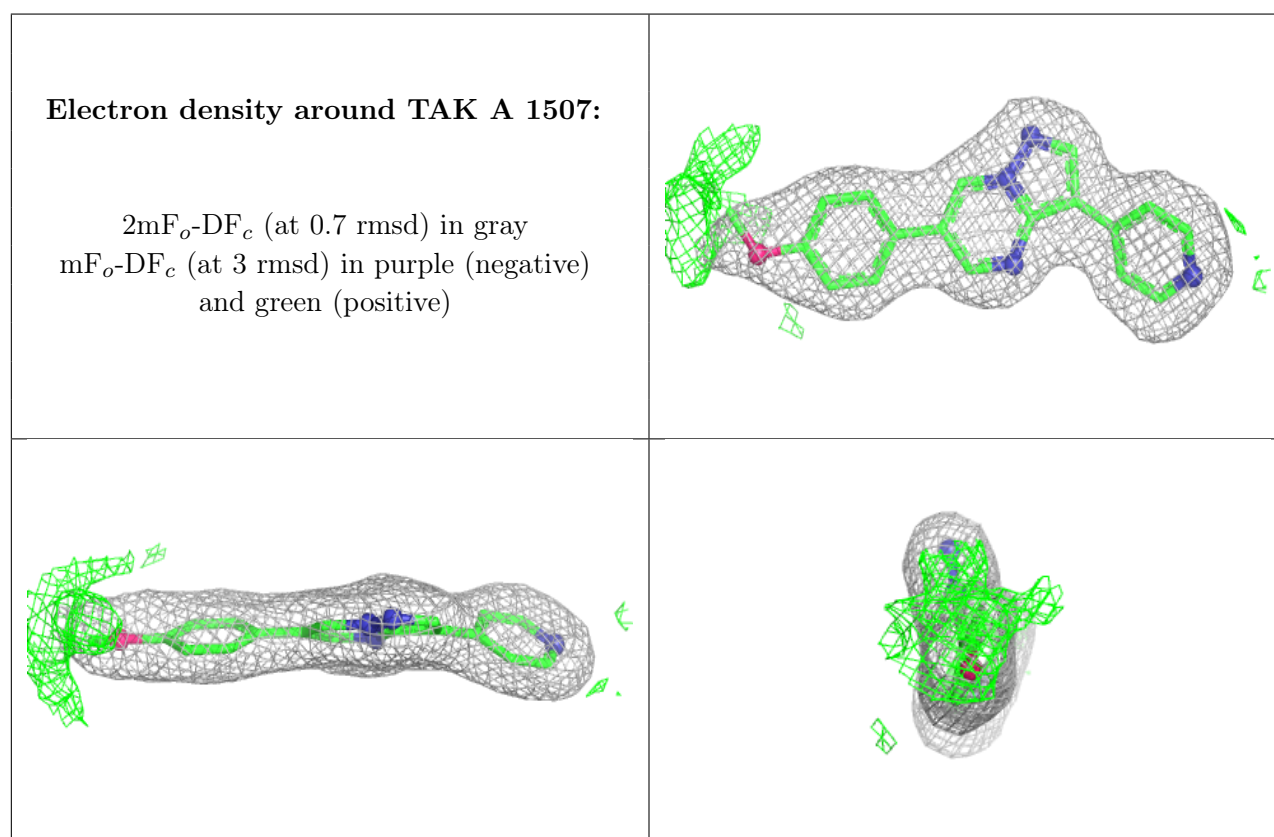
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	A	1514	4/4	0.62	0.30	64,80,83,84	0
5	EDO	A	1510	4/4	0.71	0.38	51,85,86,88	0
3	FLC	A	1505	13/13	0.75	0.20	57,80,98,98	0
5	EDO	B	1109	4/4	0.75	0.29	65,74,82,94	0
5	EDO	B	1110	4/4	0.80	0.29	36,51,69,77	0
5	EDO	A	1511	4/4	0.81	0.27	63,66,69,70	0
3	FLC	A	1506	13/13	0.84	0.23	47,81,97,97	0
3	FLC	B	1108	13/13	0.85	0.14	51,67,81,96	0
5	EDO	A	1516	4/4	0.85	0.20	45,46,50,60	0
3	FLC	A	1504	13/13	0.87	0.19	34,89,105,106	0
5	EDO	A	1512	4/4	0.87	0.25	47,56,59,74	0
5	EDO	B	1111	4/4	0.87	0.27	42,52,54,71	0
5	EDO	B	1112	4/4	0.87	0.23	47,57,59,66	0
5	EDO	A	1509	4/4	0.88	0.28	43,48,62,65	0
3	FLC	A	1502	13/13	0.89	0.16	28,53,82,102	0
5	EDO	A	1515	4/4	0.90	0.17	56,57,61,65	0
3	FLC	A	1500	13/13	0.93	0.09	36,46,57,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	1513	4/4	0.94	0.17	49,59,67,77	0
3	FLC	A	1501	13/13	0.94	0.09	36,45,60,60	0
4	TAK	A	1507	23/30	0.96	0.08	21,28,47,71	0
5	EDO	A	1508	4/4	0.96	0.09	36,42,45,45	0
3	FLC	A	1503	13/13	0.98	0.05	18,30,43,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.