



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:25 AM UTC

PDB ID : 7O7K / pdb_00007o7k
Title : Crystal structure of the human DYRK1A kinase domain bound to abemaciclib
Authors : Kaltheuner, I.H.; Anand, K.; Geyer, M.
Deposited on : 2021-04-13
Resolution : 1.82 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

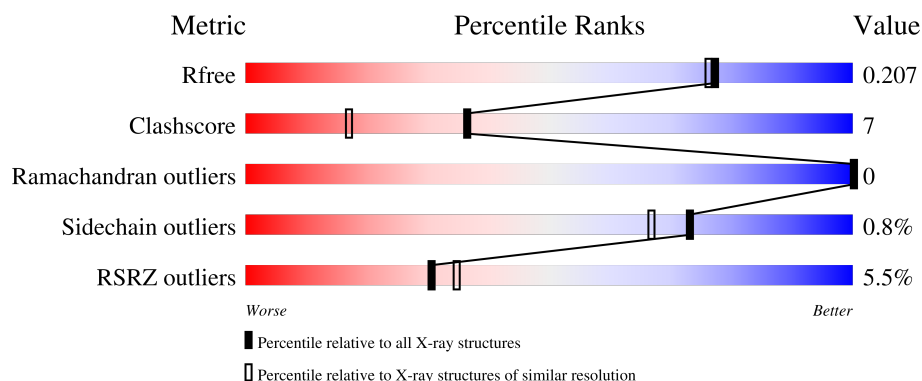
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	361	<div> <div>6%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
1	B	361	<div> <div>5%</div> <div>82%</div> <div>13%</div> <div>• •</div> </div>

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	EDO	B	509	-	-	X	-
4	EDO	B	515	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6444 atoms, of which 152 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.

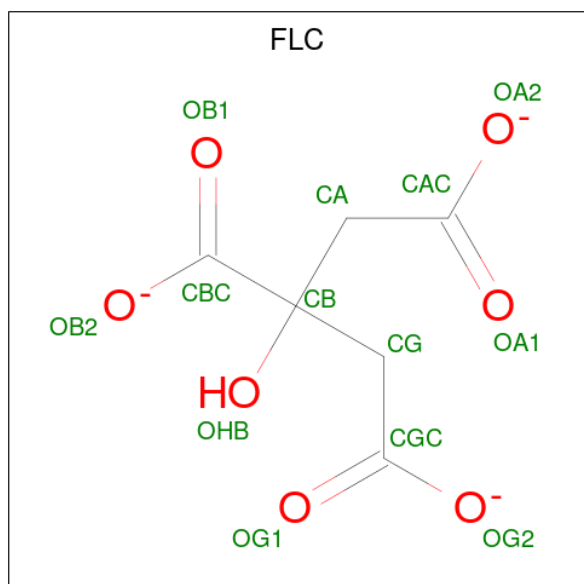
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	345	2849	1831	493	507	1	17	6	2	0
1	B	345	2996	1833	143	494	508	1	17	2	0

There are 4 discrepancies between the modelled and reference sequences:

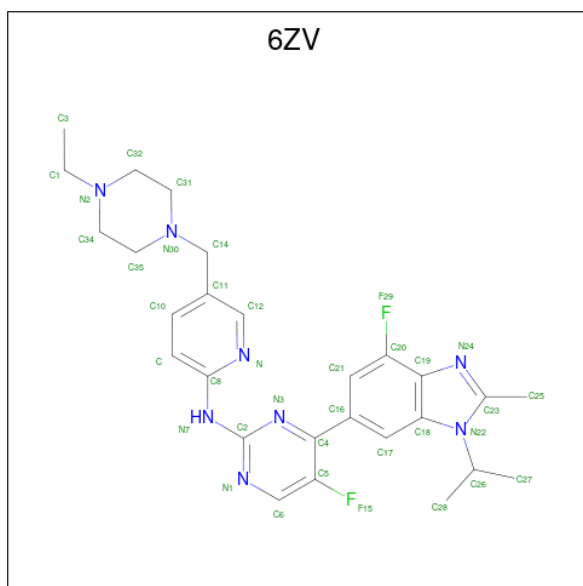
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
B	126	MET	-	expression tag	UNP Q13627

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7^-$).



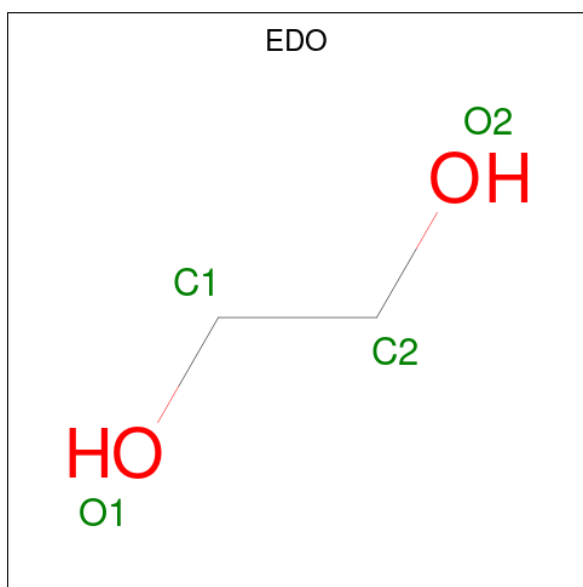
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	H	O	0
			17	6	4	7	
2	B	1	Total	C	H	O	0
			18	6	5	7	

- Molecule 3 is N-{5-[(4-ethylpiperazin-1-yl)methyl]pyridin-2-yl}-5-fluoro-4-[4-fluoro-2-methyl-1-(propan-2-yl)-1H-benzimidazol-6-yl]pyrimidin-2-amine (CCD ID: 6ZV) (formula: C₂₇H₃₂F₂N₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	F	N	0
			37	27	2	8	
3	B	1	Total	C	F	N	0
			37	27	2	8	

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



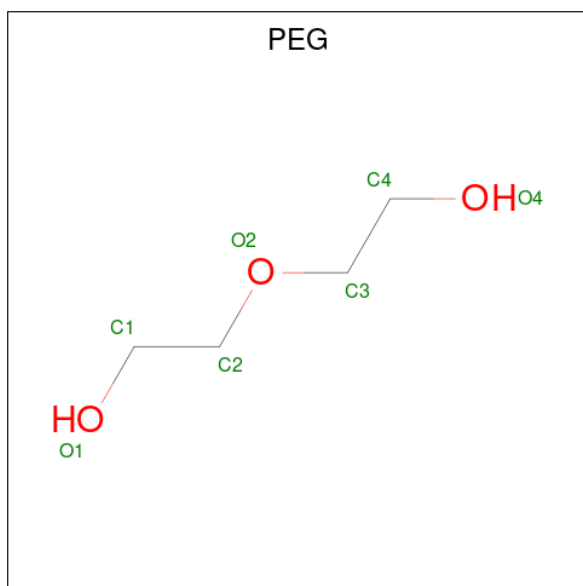
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is LITHIUM ION (CCD ID: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Li	0	0
			1	1		
6	B	1	Total	Li	0	0
			1	1		

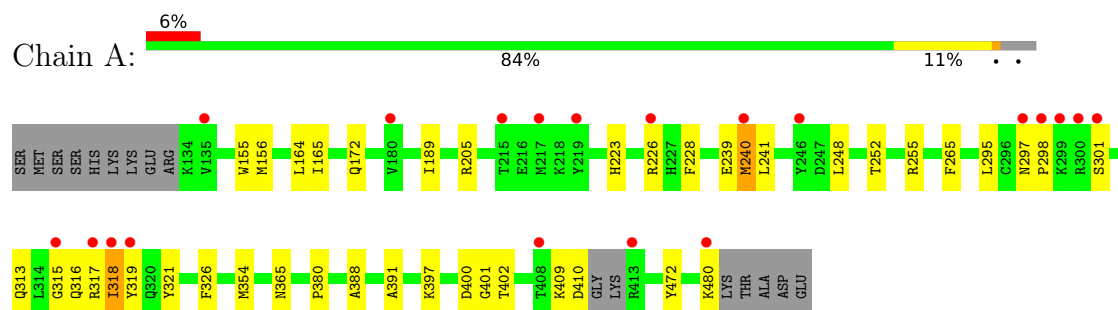
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	196	Total 196	O 196	0	0
7	B	179	Total 179	O 179	0	0

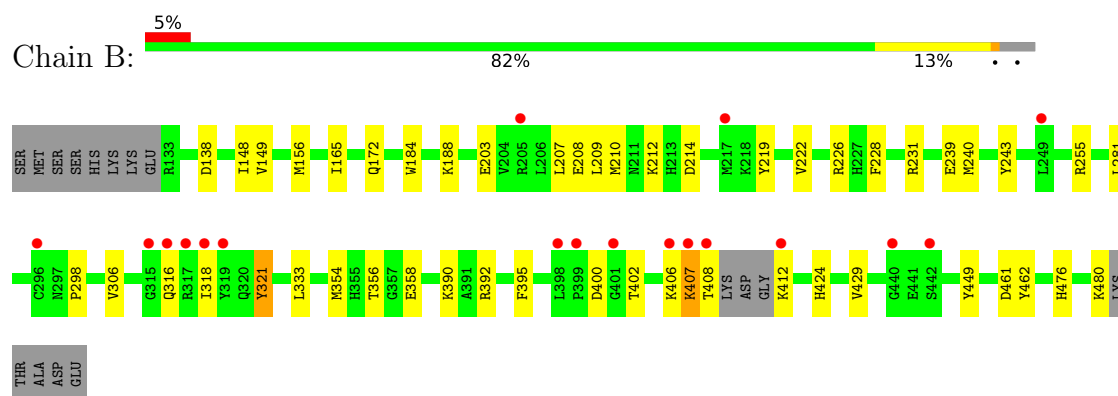
3 Residue-property plots [i](#)

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: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.70Å 109.98Å 112.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.93 – 1.82 41.93 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.93-1.82) 99.7 (41.93-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.177 , 0.205 0.181 , 0.207	Depositor DCC
R_{free} test set	4286 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6444	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6ZV, PEG, LI, PTR, FLC, 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	0.67	4/2900 (0.1%)	0.76	6/3905 (0.2%)
1	B	0.58	0/2901	0.71	3/3906 (0.1%)
All	All	0.63	4/5801 (0.1%)	0.74	9/7811 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	GLU	CD-OE2	7.15	1.39	1.25
1	A	380	PRO	CA-C	5.65	1.54	1.51
1	A	410	ASP	CG-OD1	5.60	1.35	1.25
1	A	240	MET	SD-CE	-5.34	1.66	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ASP	CB-CG-OD1	10.72	143.06	118.40
1	B	408	THR	CA-CB-OG1	8.85	122.88	109.60
1	A	409	LYS	CD-CE-NZ	-7.99	86.35	111.90
1	B	408	THR	N-CA-CB	6.47	122.50	111.50
1	A	239	GLU	CB-CG-CD	6.25	123.22	112.60
1	A	410	ASP	CB-CG-OD2	-5.81	105.04	118.40
1	A	410	ASP	OD1-CG-OD2	-5.64	109.36	122.90
1	A	409	LYS	CG-CD-CE	-5.57	98.49	111.30
1	B	408	THR	CA-C-O	-5.39	111.64	120.80

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	2849	0	2864	33	1
1	B	2853	143	2865	50	0
2	A	26	0	8	1	0
2	B	26	9	8	0	0
3	A	37	0	0	0	0
3	B	37	0	0	0	0
4	A	32	0	48	2	0
4	B	48	0	72	24	0
5	A	7	0	10	0	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
7	A	196	0	0	6	0
7	B	179	0	0	9	1
All	All	6292	152	5875	85	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 7.

All (85) 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:184:TRP:HB3	1:B:240:MET:HE3	1.39	0.98
1:A:240:MET:HE3	1:A:241:LEU:O	1.75	0.85
1:B:184:TRP:HB3	1:B:240:MET:CE	2.07	0.85
4:B:505:EDO:H11	7:B:735:HOH:O	1.79	0.82
1:B:212:LYS:HD3	7:B:671:HOH:O	1.83	0.79
1:B:149:VAL:H	4:B:509:EDO:H11	1.47	0.78
1:B:214:ASP:OD2	7:B:601:HOH:O	2.02	0.77
1:B:219:TYR:N	7:B:601:HOH:O	2.08	0.76
1:B:480:LYS:C	4:B:507:EDO:H12	2.13	0.74
1:A:298:PRO:HG2	7:A:901:HOH:O	1.89	0.72
1:B:156:MET:HE1	1:B:228:PHE:CE1	2.26	0.70
1:B:208:GLU:OE2	4:B:513:EDO:H22	1.92	0.70
1:B:400:ASP:OD2	1:B:402:THR:HG23	1.93	0.68
1:B:392:ARG:O	1:B:406:LYS:NZ	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:GLU:OE2	4:B:510:EDO:H22	1.95	0.67
1:B:480:LYS:O	4:B:507:EDO:H12	1.95	0.67
1:B:243:TYR:CD2	1:B:298:PRO:HD3	2.29	0.67
1:B:354:MET:HG3	7:B:774:HOH:O	1.95	0.66
1:A:301:SER:OG	7:A:901:HOH:O	2.13	0.66
2:A:802:FLC:OHB	6:A:813:LI:LI	1.38	0.61
1:B:424:HIS:HB3	7:B:742:HOH:O	2.02	0.60
1:B:149:VAL:H	4:B:509:EDO:C1	2.14	0.60
1:B:462:TYR:H	4:B:515:EDO:H12	1.66	0.60
1:B:243:TYR:CE2	1:B:298:PRO:HD3	2.38	0.58
1:A:326:PHE:CG	4:A:807:EDO:H11	2.38	0.57
1:B:172:GLN:OE1	4:B:509:EDO:H12	2.04	0.57
1:A:480:LYS:HE3	1:A:480:LYS:HA	1.86	0.57
1:A:400:ASP:OD1	1:A:402:THR:HG23	2.06	0.56
1:B:462:TYR:H	4:B:515:EDO:C2	2.20	0.55
1:A:326:PHE:CD2	4:A:807:EDO:H11	2.42	0.54
1:A:397:LYS:HE3	1:A:401:GLY:O	2.08	0.54
1:B:321:PTR:O	4:B:501:EDO:H11	2.08	0.53
1:B:461:ASP:HA	4:B:515:EDO:H21	1.90	0.53
4:B:512:EDO:H12	7:B:663:HOH:O	2.09	0.53
1:A:205[B]:ARG:HH11	1:A:205[B]:ARG:HG2	1.74	0.52
1:A:313:GLN:HB2	1:A:316:GLN:HG3	1.90	0.52
1:B:476:HIS:HA	4:B:514:EDO:H22	1.92	0.51
1:B:358:GLU:CD	4:B:510:EDO:H22	2.34	0.51
1:B:231:ARG:HE	4:B:508:EDO:C1	2.24	0.50
1:B:462:TYR:H	4:B:515:EDO:C1	2.23	0.50
1:A:297:ASN:N	1:A:298:PRO:HD2	2.27	0.50
1:B:188:LYS:NZ	1:B:203:GLU:OE2	2.45	0.50
1:B:356:THR:O	4:B:510:EDO:H11	2.11	0.50
1:B:184:TRP:CE3	1:B:240:MET:HE1	2.47	0.49
1:B:226:ARG:HA	4:B:513:EDO:O2	2.13	0.48
1:A:365:ASN:HB2	1:B:138:ASP:OD1	2.14	0.48
1:B:333:LEU:O	1:B:390:LYS:HE3	2.14	0.48
1:A:265:PHE:HD2	1:A:354:MET:HE3	1.79	0.47
1:B:239:GLU:HG2	7:B:606:HOH:O	2.15	0.47
1:A:205[B]:ARG:HG2	1:A:205[B]:ARG:NH1	2.30	0.47
1:B:222:VAL:HG21	1:B:306:VAL:CG1	2.43	0.47
1:B:212:LYS:HA	1:B:212:LYS:HD2	1.80	0.47
1:B:462:TYR:N	4:B:515:EDO:H12	2.30	0.46
1:B:208:GLU:OE2	4:B:513:EDO:C2	2.61	0.46
1:A:354:MET:HB3	1:A:354:MET:HE2	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:PHE:C	1:B:406:LYS:HG3	2.40	0.46
1:A:156:MET:HE1	1:A:228:PHE:CE1	2.51	0.46
1:A:265:PHE:HD2	1:A:354:MET:CE	2.29	0.46
1:A:226[A]:ARG:HG3	7:A:1043:HOH:O	2.16	0.46
1:B:148:ILE:HA	4:B:509:EDO:H11	1.98	0.45
1:B:207:LEU:HD23	1:B:210:MET:HE3	1.98	0.45
1:A:252:THR:O	1:A:255:ARG:HG2	2.17	0.45
1:A:248:LEU:HB2	1:A:295:LEU:HD11	1.99	0.44
1:B:407:LYS:HD3	1:B:407:LYS:HA	1.58	0.44
1:A:155:TRP:HH2	1:A:189:ILE:CD1	2.31	0.44
1:A:317:ARG:HD2	1:A:319:TYR:CE2	2.53	0.44
1:B:400:ASP:OD2	1:B:402:THR:CG2	2.65	0.43
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.83	0.43
1:A:164:LEU:HD11	1:A:172:GLN:HB3	2.00	0.43
1:A:223:HIS:HB2	7:A:1044:HOH:O	2.19	0.43
1:A:318:ILE:HG22	1:A:318:ILE:O	2.19	0.43
1:A:156:MET:HE3	1:A:156:MET:HB2	1.89	0.42
1:B:231:ARG:HE	4:B:508:EDO:H11	1.85	0.42
1:A:316:GLN:N	7:A:910:HOH:O	2.52	0.42
1:A:388:ALA:HB3	1:A:391:ALA:HB2	2.02	0.42
1:B:209:LEU:HG	1:B:281:LEU:CD2	2.49	0.42
1:B:149:VAL:N	4:B:509:EDO:H11	2.26	0.42
1:B:390:LYS:HE2	7:B:710:HOH:O	2.19	0.41
1:A:315:GLY:C	7:A:910:HOH:O	2.63	0.41
1:B:165:ILE:HD13	1:B:165:ILE:HG21	1.85	0.40
1:B:429:VAL:HG22	1:B:449:TYR:HB3	2.03	0.40
1:A:480:LYS:HE3	1:A:480:LYS:CA	2.50	0.40
1:A:165:ILE:HD13	1:A:165:ILE:HG21	1.80	0.40
1:A:318:ILE:N	1:A:318:ILE:HD12	2.37	0.40
1:A:480:LYS:HA	1:A:480:LYS:CE	2.49	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)
1:A:472:TYR:OH	7:B:756:HOH:O[3_655]	2.17	0.03

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	342/361 (95%)	330 (96%)	12 (4%)	0	100	100
1	B	342/361 (95%)	330 (96%)	12 (4%)	0	100	100
All	All	684/722 (95%)	660 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/320 (96%)	307 (100%)	1 (0%)	86	84
1	B	308/320 (96%)	304 (99%)	4 (1%)	61	50
All	All	616/640 (96%)	611 (99%)	5 (1%)	73	67

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

Mol	Chain	Res	Type
1	A	318	ILE
1	B	316	GLN
1	B	318	ILE
1	B	407	LYS
1	B	412	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	251	ASN
1	A	371	ASN
1	B	198	ASN
1	B	475	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PTR	B	321	1	15,16,17	1.11	1 (6%)	17,22,24	1.06	1 (5%)
1	PTR	A	321	1	15,16,17	1.03	1 (6%)	17,22,24	1.12	1 (5%)

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
1	PTR	B	321	1	-	1/10/11/13	0/1/1/1
1	PTR	A	321	1	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	PTR	P-OH	3.10	1.65	1.59
1	B	321	PTR	P-OH	2.78	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	PTR	CD2-CG-CD1	2.50	121.95	118.23
1	B	321	PTR	CD2-CG-CD1	2.03	121.25	118.23

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	321	PTR	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	321	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	$\# Z > 2$
4	EDO	B	507	-	3,3,3	0.45	0	2,2,2	0.57	0
4	EDO	B	501	-	3,3,3	0.42	0	2,2,2	0.45	0
4	EDO	B	511	-	3,3,3	0.48	0	2,2,2	0.52	0
4	EDO	B	506	-	3,3,3	0.46	0	2,2,2	0.25	0
4	EDO	B	505	-	3,3,3	0.50	0	2,2,2	0.17	0
2	FLC	A	802	6	12,12,12	1.48	2 (16%)	17,17,17	2.13	5 (29%)
4	EDO	B	513	-	3,3,3	0.54	0	2,2,2	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FLC	B	503	6	12,12,12	1.17	0	17,17,17	2.09	6 (35%)
2	FLC	B	502	-	12,12,12	0.93	0	17,17,17	1.36	2 (11%)
4	EDO	A	812	-	3,3,3	0.44	0	2,2,2	0.32	0
4	EDO	B	510	-	3,3,3	0.42	0	2,2,2	0.64	0
4	EDO	B	512	-	3,3,3	0.47	0	2,2,2	0.19	0
4	EDO	A	807	-	3,3,3	0.43	0	2,2,2	0.56	0
4	EDO	A	808	-	3,3,3	0.43	0	2,2,2	0.90	0
4	EDO	B	508	-	3,3,3	0.46	0	2,2,2	0.49	0
3	6ZV	A	803	-	39,41,41	2.57	11 (28%)	48,59,59	2.01	12 (25%)
4	EDO	A	809	-	3,3,3	0.45	0	2,2,2	0.38	0
4	EDO	A	806	-	3,3,3	0.48	0	2,2,2	0.61	0
4	EDO	A	810	-	3,3,3	0.49	0	2,2,2	0.64	0
4	EDO	A	804	-	3,3,3	0.48	0	2,2,2	0.71	0
4	EDO	B	514	-	3,3,3	0.41	0	2,2,2	0.67	0
3	6ZV	B	504	-	39,41,41	2.70	13 (33%)	48,59,59	1.66	8 (16%)
5	PEG	A	811	-	6,6,6	0.81	0	5,5,5	0.79	0
4	EDO	B	509	-	3,3,3	0.50	0	2,2,2	0.43	0
2	FLC	A	801	-	12,12,12	1.51	3 (25%)	17,17,17	1.39	1 (5%)
4	EDO	A	805	-	3,3,3	0.43	0	2,2,2	0.23	0
4	EDO	B	515	-	3,3,3	0.42	0	2,2,2	0.22	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
4	EDO	B	507	-	-	1/1/1/1	-
4	EDO	B	501	-	-	1/1/1/1	-
4	EDO	B	511	-	-	1/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
2	FLC	A	802	6	-	0/16/16/16	-
4	EDO	B	513	-	-	0/1/1/1	-
2	FLC	B	503	6	-	2/16/16/16	-
2	FLC	B	502	-	-	0/16/16/16	-
4	EDO	A	812	-	-	1/1/1/1	-
4	EDO	B	510	-	-	0/1/1/1	-
4	EDO	B	512	-	-	1/1/1/1	-
4	EDO	A	807	-	-	1/1/1/1	-
4	EDO	A	808	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	508	-	-	1/1/1/1	-
3	6ZV	A	803	-	-	9/18/28/28	0/5/5/5
4	EDO	A	809	-	-	1/1/1/1	-
4	EDO	A	806	-	-	1/1/1/1	-
4	EDO	A	810	-	-	1/1/1/1	-
4	EDO	A	804	-	-	0/1/1/1	-
4	EDO	B	514	-	-	1/1/1/1	-
3	6ZV	B	504	-	-	8/18/28/28	0/5/5/5
5	PEG	A	811	-	-	1/4/4/4	-
4	EDO	B	509	-	-	0/1/1/1	-
2	FLC	A	801	-	-	2/16/16/16	-
4	EDO	A	805	-	-	0/1/1/1	-
4	EDO	B	515	-	-	0/1/1/1	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	6ZV	C16-C4	8.19	1.58	1.49
3	B	504	6ZV	C16-C4	7.81	1.57	1.49
3	B	504	6ZV	C23-N24	6.72	1.40	1.31
3	B	504	6ZV	C8-N7	6.63	1.50	1.38
3	A	803	6ZV	C23-N24	6.25	1.40	1.31
3	A	803	6ZV	C8-N7	5.77	1.48	1.38
3	B	504	6ZV	C2-N7	5.54	1.48	1.36
3	A	803	6ZV	C2-N7	5.15	1.47	1.36
3	A	803	6ZV	C21-C16	3.81	1.46	1.39
3	B	504	6ZV	C19-N24	3.72	1.46	1.39
3	B	504	6ZV	C21-C16	3.51	1.45	1.39
3	A	803	6ZV	C18-N22	-3.20	1.35	1.40
3	B	504	6ZV	C-C8	3.17	1.46	1.39
3	A	803	6ZV	C19-N24	3.08	1.44	1.39
3	B	504	6ZV	C2-N3	3.02	1.43	1.34
3	A	803	6ZV	C2-N3	2.87	1.42	1.34
3	A	803	6ZV	C-C8	2.77	1.46	1.39
3	B	504	6ZV	C2-N1	2.75	1.38	1.34
2	A	802	FLC	OG1-CGC	2.72	1.31	1.22
3	A	803	6ZV	C17-C18	2.51	1.43	1.39
3	B	504	6ZV	C17-C18	2.46	1.43	1.39
2	A	801	FLC	OG2-CGC	-2.39	1.22	1.30
3	B	504	6ZV	C8-N	2.38	1.38	1.34
2	A	802	FLC	OHB-CB	-2.31	1.38	1.43
3	B	504	6ZV	C18-N22	-2.25	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FLC	OA1-CAC	2.25	1.29	1.22
3	B	504	6ZV	C6-C5	2.17	1.41	1.37
2	A	801	FLC	CB-CBC	-2.16	1.51	1.53
3	A	803	6ZV	C2-N1	2.10	1.37	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	6ZV	C16-C21-C20	-5.87	114.97	119.61
2	A	802	FLC	OHB-CB-CBC	-5.17	101.63	108.96
3	B	504	6ZV	C14-N30-C31	-4.80	100.73	111.07
2	B	503	FLC	OHB-CB-CBC	-4.53	102.53	108.96
3	A	803	6ZV	C21-C16-C17	4.47	124.88	118.35
3	A	803	6ZV	N1-C2-N3	-4.28	122.28	126.42
3	A	803	6ZV	C14-C11-C10	4.15	128.39	120.75
2	A	802	FLC	OB2-CBC-CB	3.82	120.48	113.14
3	B	504	6ZV	C18-N22-C23	3.76	109.24	106.75
3	A	803	6ZV	C11-C14-N30	-3.69	105.59	113.15
3	B	504	6ZV	C14-N30-C35	-3.51	103.51	111.07
2	B	503	FLC	OB2-CBC-CB	3.46	119.78	113.14
3	B	504	6ZV	C16-C4-N3	3.39	119.72	115.10
3	B	504	6ZV	C16-C21-C20	-3.30	117.00	119.61
2	A	801	FLC	OHB-CB-CBC	-3.28	104.30	108.96
3	B	504	6ZV	C12-N-C8	3.23	120.86	117.83
3	A	803	6ZV	C14-C11-C12	-3.14	113.77	120.87
2	B	503	FLC	CG-CB-CBC	-3.01	103.38	110.03
3	A	803	6ZV	C28-C26-N22	-2.99	106.89	111.11
3	A	803	6ZV	C18-N22-C23	2.94	108.69	106.75
2	B	502	FLC	OB2-CBC-CB	2.73	118.38	113.14
2	A	802	FLC	CG-CB-CBC	-2.72	104.01	110.03
3	B	504	6ZV	N7-C2-N1	2.70	123.95	116.29
3	A	803	6ZV	C16-C17-C18	-2.68	115.28	119.47
3	B	504	6ZV	N1-C2-N3	-2.62	123.89	126.42
3	A	803	6ZV	C6-N1-C2	2.59	119.36	115.81
2	B	503	FLC	OG2-CGC-CG	2.54	122.40	114.35
3	A	803	6ZV	C12-N-C8	2.33	120.02	117.83
2	A	802	FLC	OG2-CGC-OG1	-2.32	117.38	123.33
2	A	802	FLC	OB1-CBC-CB	-2.25	117.73	122.09
2	B	502	FLC	CG-CB-CBC	2.22	114.95	110.03
3	A	803	6ZV	C18-N22-C26	2.05	129.84	126.55
2	B	503	FLC	OB1-CBC-CB	-2.05	118.13	122.09
2	B	503	FLC	CA-CB-CBC	2.04	114.55	110.03

There are no chirality outliers.

All (35) torsion outliers are listed below:

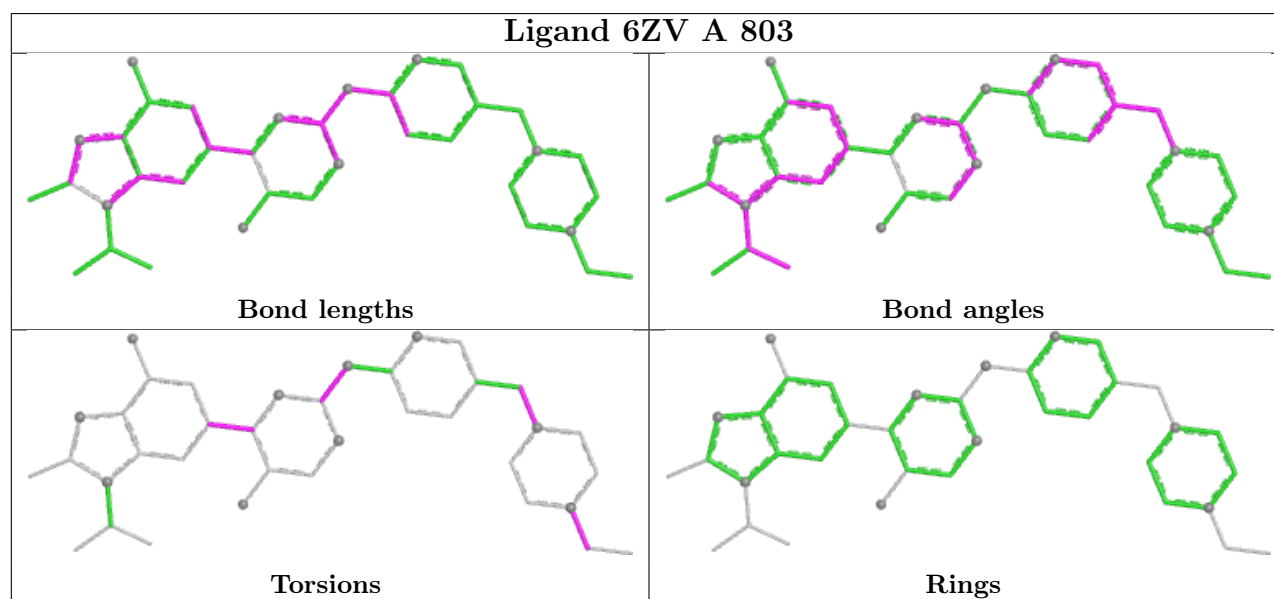
Mol	Chain	Res	Type	Atoms
3	B	504	6ZV	N3-C2-N7-C8
3	A	803	6ZV	N3-C2-N7-C8
3	B	504	6ZV	N1-C2-N7-C8
3	A	803	6ZV	N1-C2-N7-C8
4	A	808	EDO	O1-C1-C2-O2
4	B	507	EDO	O1-C1-C2-O2
4	B	511	EDO	O1-C1-C2-O2
3	A	803	6ZV	C3-C1-N2-C32
3	A	803	6ZV	C3-C1-N2-C34
3	B	504	6ZV	C3-C1-N2-C32
3	B	504	6ZV	C3-C1-N2-C34
4	A	809	EDO	O1-C1-C2-O2
3	B	504	6ZV	C21-C16-C4-N3
3	B	504	6ZV	C17-C16-C4-N3
3	B	504	6ZV	C21-C16-C4-C5
3	A	803	6ZV	C21-C16-C4-N3
4	A	810	EDO	O1-C1-C2-O2
3	A	803	6ZV	C17-C16-C4-N3
3	A	803	6ZV	C21-C16-C4-C5
4	A	807	EDO	O1-C1-C2-O2
3	A	803	6ZV	C11-C14-N30-C35
4	B	514	EDO	O1-C1-C2-O2
2	B	503	FLC	CB-CG-CGC-OG1
2	B	503	FLC	CB-CG-CGC-OG2
3	A	803	6ZV	C17-C16-C4-C5
2	A	801	FLC	CB-CA-CAC-OA2
3	B	504	6ZV	C17-C16-C4-C5
4	B	506	EDO	O1-C1-C2-O2
2	A	801	FLC	CB-CA-CAC-OA1
5	A	811	PEG	O1-C1-C2-O2
4	B	508	EDO	O1-C1-C2-O2
4	B	512	EDO	O1-C1-C2-O2
4	A	806	EDO	O1-C1-C2-O2
4	A	812	EDO	O1-C1-C2-O2
4	B	501	EDO	O1-C1-C2-O2

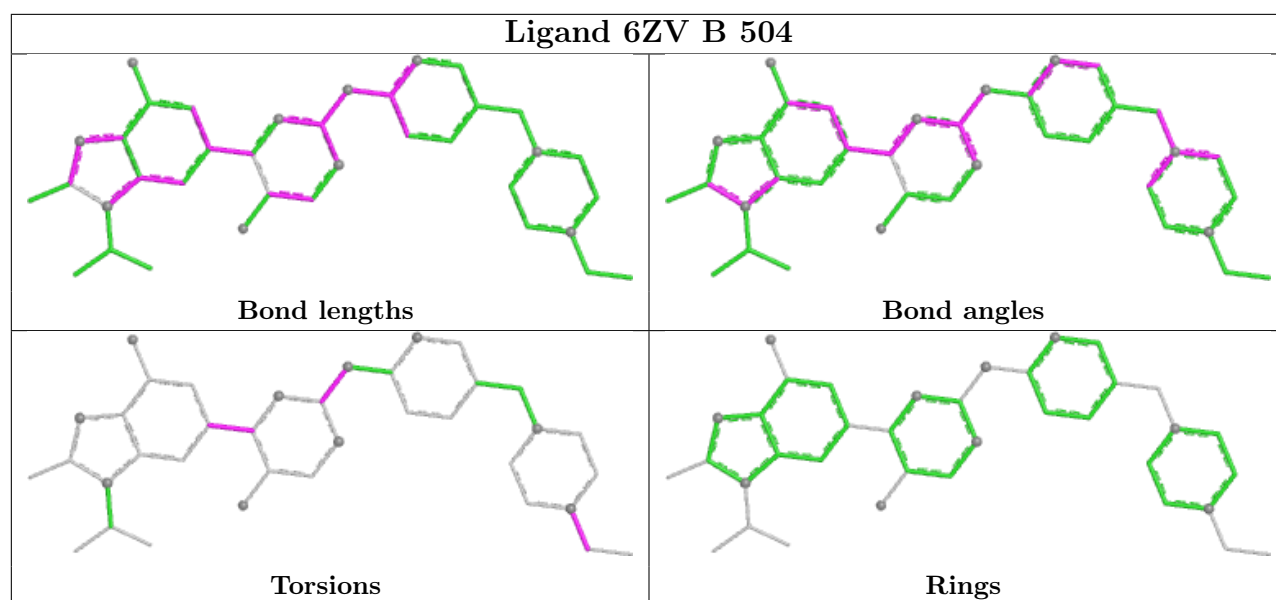
There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	507	EDO	2	0
4	B	501	EDO	1	0
4	B	505	EDO	1	0
2	A	802	FLC	1	0
4	B	513	EDO	3	0
4	B	510	EDO	3	0
4	B	512	EDO	1	0
4	A	807	EDO	2	0
4	B	508	EDO	2	0
4	B	514	EDO	1	0
4	B	509	EDO	5	0
4	B	515	EDO	5	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	344/361 (95%)	0.16	20 (5%) 29 32	21, 43, 70, 102	4 (1%)
1	B	344/361 (95%)	0.29	18 (5%) 33 37	19, 46, 70, 95	6 (1%)
All	All	688/722 (95%)	0.23	38 (5%) 30 35	19, 44, 71, 102	10 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	408	THR	4.9
1	A	318	ILE	4.1
1	B	318	ILE	3.6
1	A	298	PRO	3.6
1	A	300	ARG	3.6
1	B	398	LEU	3.5
1	A	408	THR	3.4
1	B	319	TYR	3.3
1	B	316	GLN	3.2
1	B	205[A]	ARG	3.1
1	B	440	GLY	2.8
1	A	219	TYR	2.8
1	B	317	ARG	2.8
1	A	413	ARG	2.7
1	B	296	CYS	2.6
1	A	226[A]	ARG	2.5
1	A	480	LYS	2.5
1	B	315	GLY	2.5
1	A	299	LYS	2.5
1	B	399	PRO	2.5
1	B	407	LYS	2.4
1	A	246	TYR	2.4
1	A	319	TYR	2.4
1	A	217	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	406	LYS	2.3
1	A	240	MET	2.2
1	B	217	MET	2.2
1	A	315	GLY	2.2
1	A	135	VAL	2.2
1	B	249	LEU	2.2
1	B	401	GLY	2.2
1	A	317	ARG	2.2
1	A	301	SER	2.1
1	A	215	THR	2.1
1	B	442	SER	2.1
1	B	412	LYS	2.1
1	A	297	ASN	2.1
1	A	180	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	A	321	16/17	0.97	0.07	36,43,50,51	0
1	PTR	B	321	16/17	0.97	0.07	35,40,48,51	0

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
4	EDO	B	506	4/4	0.69	0.17	60,62,62,65	0
4	EDO	B	510	4/4	0.69	0.16	65,67,72,83	0

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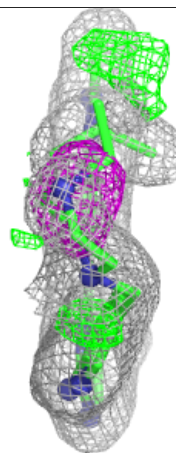
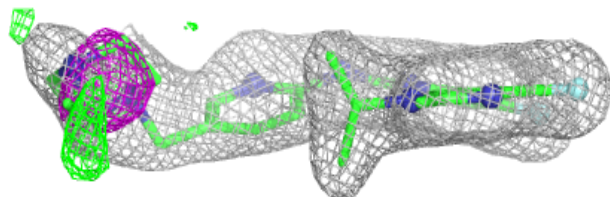
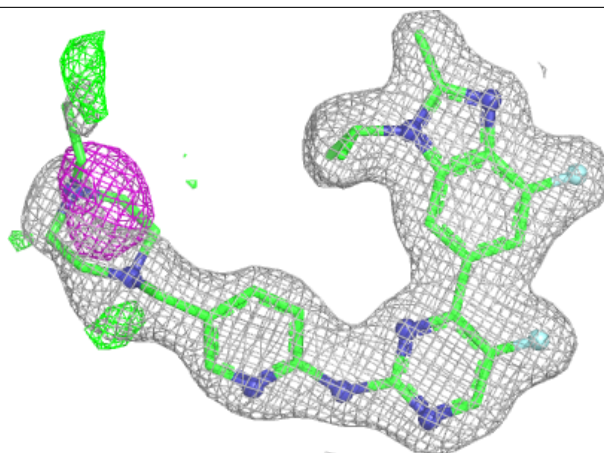
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	A	811	7/7	0.69	0.17	62,68,75,76	0
4	EDO	B	513	4/4	0.73	0.17	47,54,54,58	0
4	EDO	B	507	4/4	0.73	0.14	80,81,86,88	0
4	EDO	B	512	4/4	0.75	0.14	62,63,67,67	0
4	EDO	B	508	4/4	0.76	0.13	61,64,67,73	0
4	EDO	A	805	4/4	0.79	0.16	67,68,74,77	0
4	EDO	B	514	4/4	0.81	0.14	47,51,57,59	0
4	EDO	A	807	4/4	0.81	0.15	40,51,58,65	0
4	EDO	A	808	4/4	0.82	0.15	52,53,63,66	0
4	EDO	A	809	4/4	0.82	0.15	52,53,61,62	0
4	EDO	A	810	4/4	0.86	0.14	49,52,57,63	0
4	EDO	B	509	4/4	0.87	0.11	37,55,59,66	0
4	EDO	A	804	4/4	0.88	0.14	51,53,55,56	0
4	EDO	B	515	4/4	0.88	0.12	46,47,55,61	0
4	EDO	B	511	4/4	0.88	0.16	52,58,59,64	0
4	EDO	A	806	4/4	0.90	0.11	48,52,53,62	0
4	EDO	A	812	4/4	0.92	0.13	49,51,52,52	0
4	EDO	B	505	4/4	0.93	0.11	42,47,51,65	0
4	EDO	B	501	4/4	0.93	0.11	45,46,49,54	0
3	6ZV	B	504	37/37	0.94	0.10	30,35,65,67	0
2	FLC	B	502	13/13	0.96	0.06	33,38,46,48	0
2	FLC	B	503	13/13	0.96	0.06	31,38,45,45	0
3	6ZV	A	803	37/37	0.96	0.09	29,35,62,68	0
2	FLC	A	801	13/13	0.96	0.06	30,33,38,39	0
2	FLC	A	802	13/13	0.96	0.06	27,33,38,43	0
6	LI	B	516	1/1	0.96	0.11	32,32,32,32	0
6	LI	A	813	1/1	0.99	0.13	28,28,28,28	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.

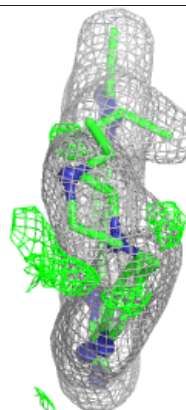
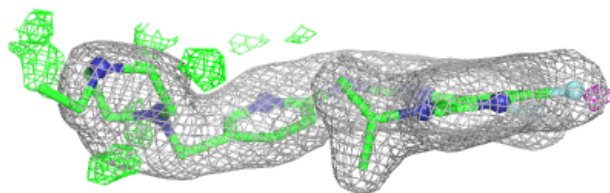
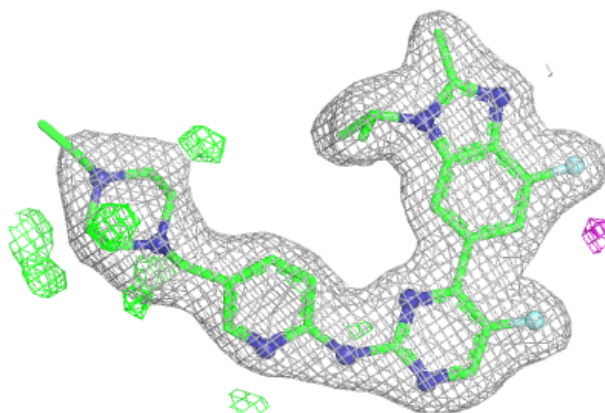
Electron density around 6ZV B 504:

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



Electron density around 6ZV A 803:

$2mF_o-DF_c$ (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.