wwPDB X-ray Structure Validation Summary Report (i)

Nov 4, 2026 – 08:10 PM EST

PDB ID	:	9Z3M / pdb_00009z3m
Title	:	Complex of phosphorylated p38-alpha and MK2 with a molecular glue
Authors	:	Bell, J.A.
Deposited on	:	2025-11-07
Resolution	:	2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

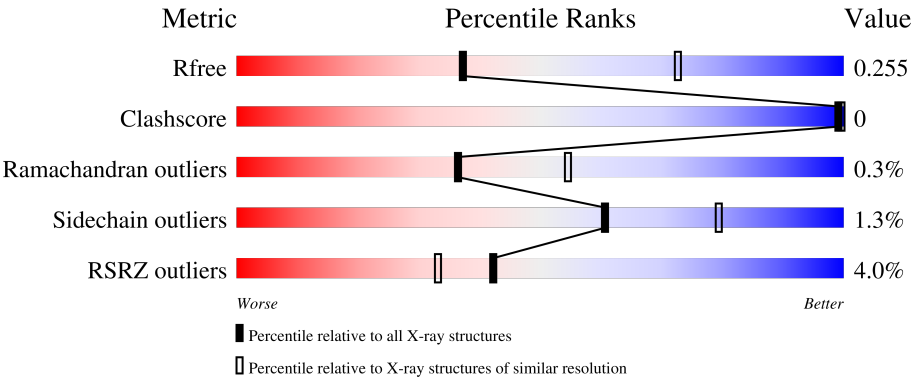
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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.



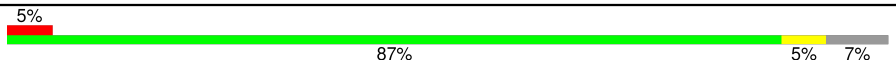
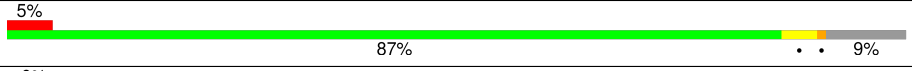
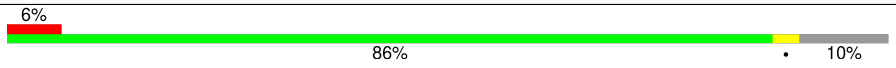
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 <=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	363	91% 6%
1	B	363	5% 90% 6%
1	C	363	4% 88% 5% 7%
1	D	363	90% 7%
2	E	363	3% 87% 8%

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Mol	Chain	Length	Quality of chain
2	F	363	
2	G	363	
2	H	363	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 45515 atoms, of which 22950 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 Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	351	Total	C	H	N	O	P	S	0	0	0
			5667	1813	2822	483	533	3	13			
1	B	351	Total	C	H	N	O	P	S	0	0	0
			5668	1813	2823	483	533	3	13			
1	C	338	Total	C	H	N	O	P	S	0	0	0
			5466	1752	2732	465	504	1	12			
1	D	351	Total	C	H	N	O	P	S	0	0	0
			5667	1813	2822	483	533	3	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q16539
A	-1	GLY	-	expression tag	UNP Q16539
A	0	GLY	-	expression tag	UNP Q16539
B	-2	GLY	-	expression tag	UNP Q16539
B	-1	GLY	-	expression tag	UNP Q16539
B	0	GLY	-	expression tag	UNP Q16539
C	-2	GLY	-	expression tag	UNP Q16539
C	-1	GLY	-	expression tag	UNP Q16539
C	0	GLY	-	expression tag	UNP Q16539
D	-2	GLY	-	expression tag	UNP Q16539
D	-1	GLY	-	expression tag	UNP Q16539
D	0	GLY	-	expression tag	UNP Q16539

- Molecule 2 is a protein called MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	333	Total	C	H	N	O	S	0	0	0
			5461	1723	2751	469	499	19			
2	F	336	Total	C	H	N	O	S	0	0	0
			5500	1737	2770	472	502	19			

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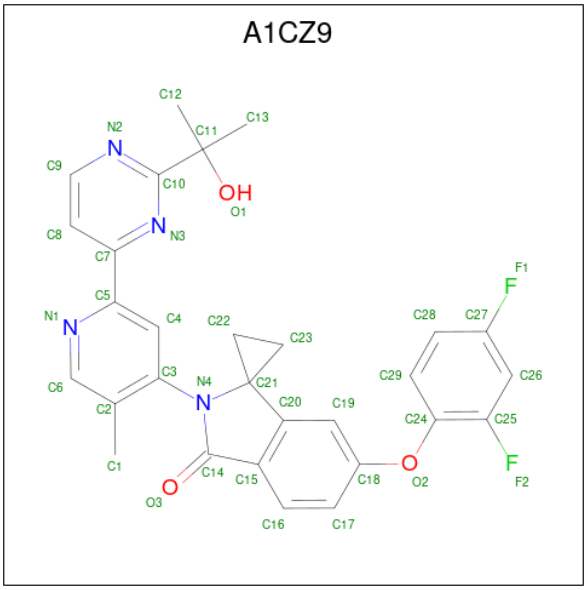
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	332	Total	C	H	N	O	S	0	0	0
			5428	1715	2740	459	495	19			
2	H	326	Total	C	H	N	O	S	0	0	0
			5355	1694	2698	457	488	18			

There are 12 discrepancies between the modelled and reference sequences:

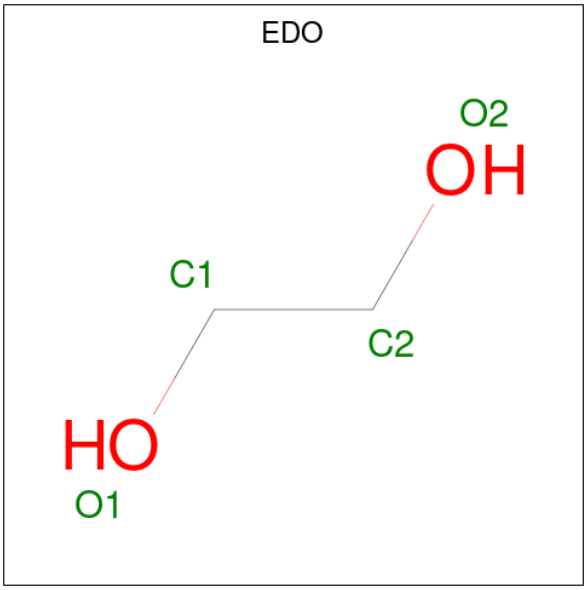
Chain	Residue	Modelled	Actual	Comment	Reference
E	38	GLY	-	expression tag	UNP P49137
E	39	GLY	-	expression tag	UNP P49137
E	40	GLY	-	expression tag	UNP P49137
F	38	GLY	-	expression tag	UNP P49137
F	39	GLY	-	expression tag	UNP P49137
F	40	GLY	-	expression tag	UNP P49137
G	38	GLY	-	expression tag	UNP P49137
G	39	GLY	-	expression tag	UNP P49137
G	40	GLY	-	expression tag	UNP P49137
H	38	GLY	-	expression tag	UNP P49137
H	39	GLY	-	expression tag	UNP P49137
H	40	GLY	-	expression tag	UNP P49137

- Molecule 3 is 6'-(2,4-difluorophenoxy)-2'-{2-[2-(2-hydroxypropan-2-yl)pyrimidin-4-yl]-5-methylpyridin-4-yl}spiro[cyclopropane-1,1'-isoindol]-3'(2'H)-one (CCD ID: A1CZ9) (formula: $C_{29}H_{24}F_2N_4O_3$) (labeled as "Ligand of Interest" by depositor).



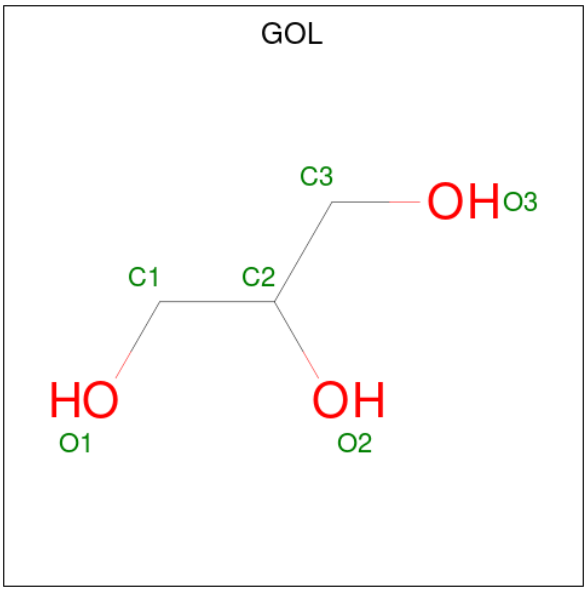
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	0	0
			62	29	2	24	4	3		
3	B	1	Total	C	F	H	N	O	0	0
			62	29	2	24	4	3		
3	C	1	Total	C	F	H	N	O	0	0
			62	29	2	24	4	3		
3	D	1	Total	C	F	H	N	O	0	0
			62	29	2	24	4	3		

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



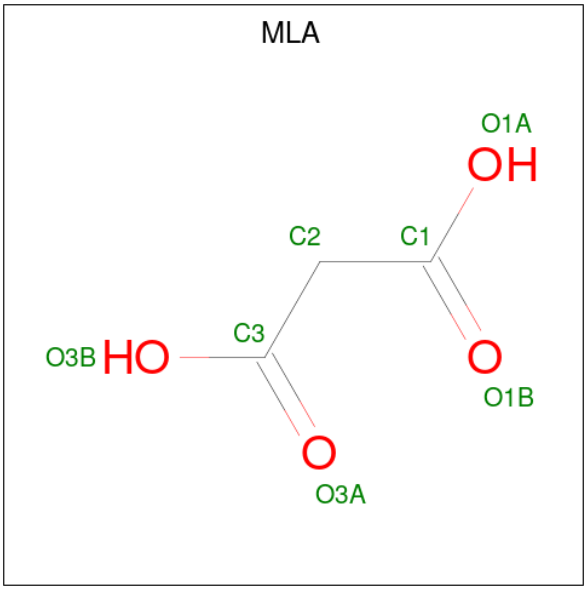
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	H	O	0	0
			11	3	4	4		

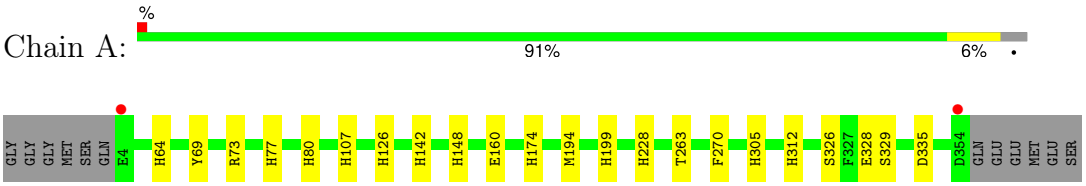
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	74	Total H O 222 148 74	0	0
7	B	36	Total H O 108 72 36	0	0
7	C	39	Total H O 117 78 39	0	0
7	D	49	Total H O 147 98 49	0	0
7	E	43	Total H O 129 86 43	0	0
7	F	37	Total H O 111 74 37	0	0
7	G	18	Total H O 54 36 18	0	0
7	H	34	Total H O 102 68 34	0	0

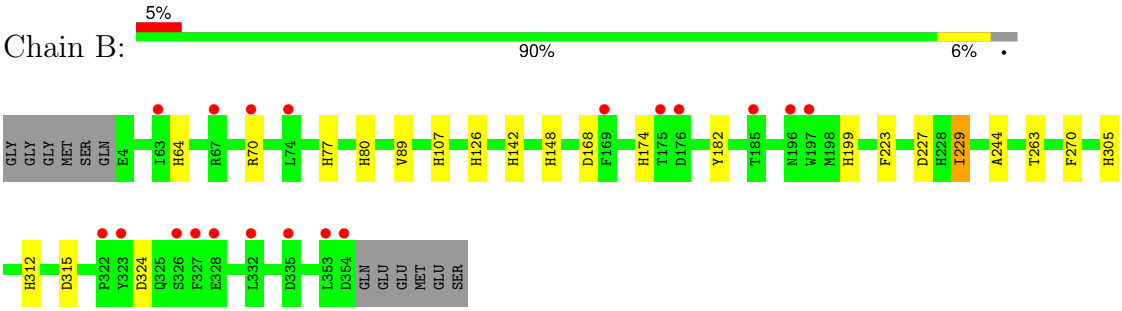
3 Residue-property plots (i)

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.

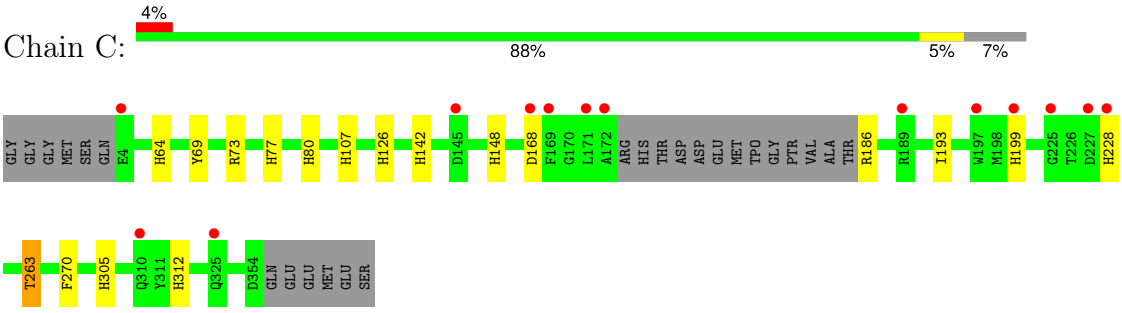
• Molecule 1: Mitogen-activated protein kinase 14



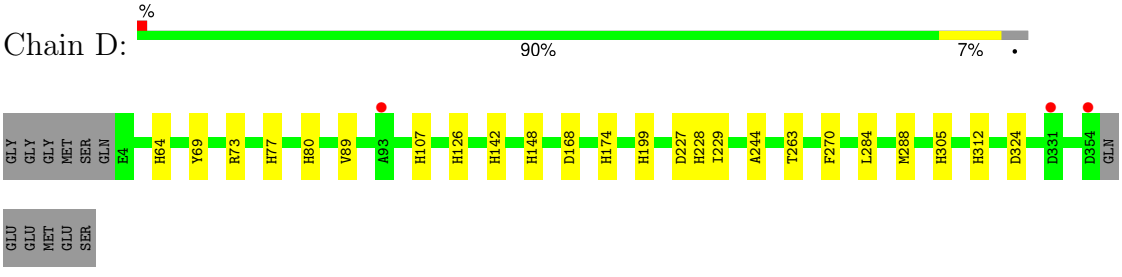
• Molecule 1: Mitogen-activated protein kinase 14



• Molecule 1: Mitogen-activated protein kinase 14

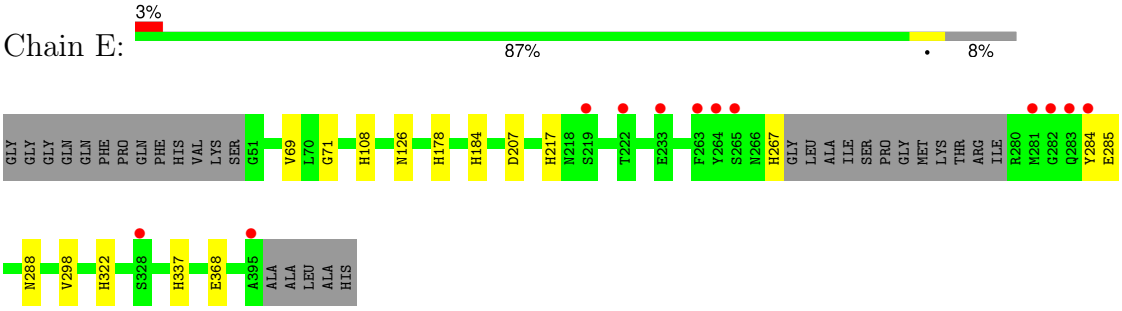


• Molecule 1: Mitogen-activated protein kinase 14



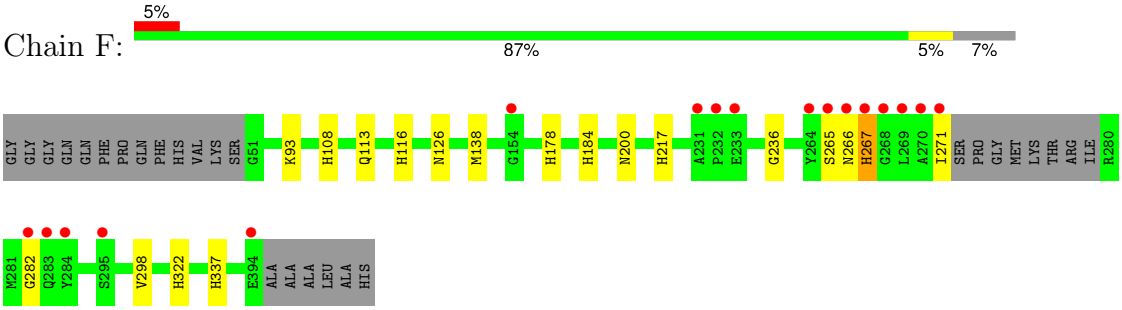
• Molecule 2: MAP kinase-activated protein kinase 2

Chain E:



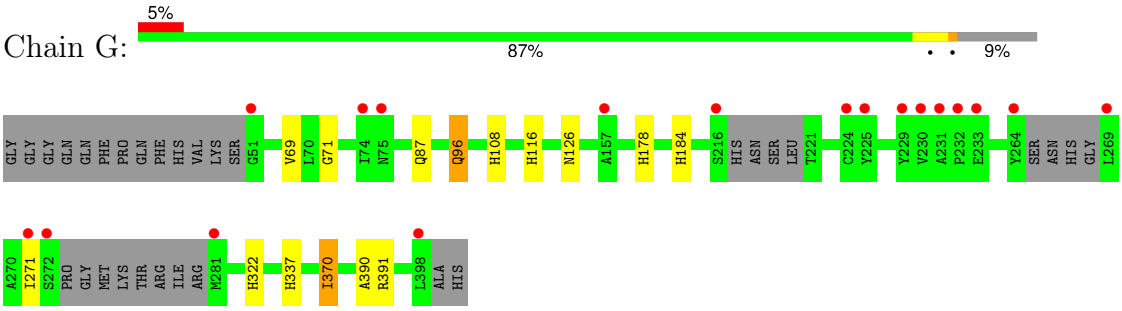
• Molecule 2: MAP kinase-activated protein kinase 2

Chain F:



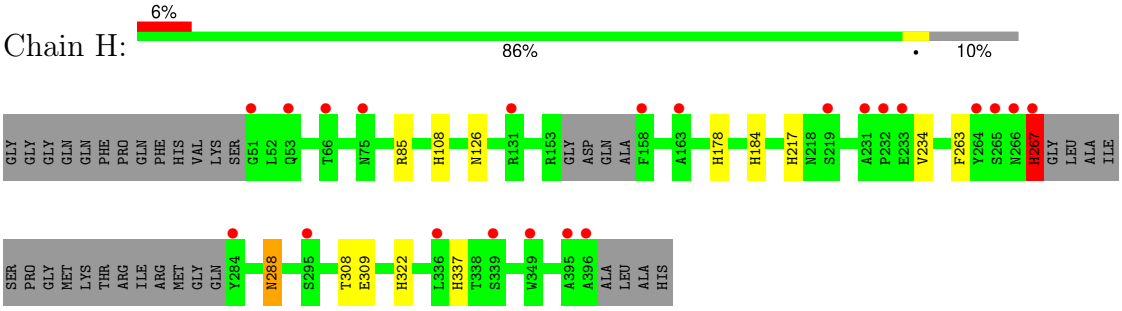
• Molecule 2: MAP kinase-activated protein kinase 2

Chain G:



• Molecule 2: MAP kinase-activated protein kinase 2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.68Å 229.77Å 127.38Å 90.00° 103.90° 90.00°	Depositor
Resolution (Å)	49.45 – 2.85 49.45 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.45-2.85) 99.9 (49.45-2.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.86Å)	Xtriage
Refinement program	PRIME-X	Depositor
R, R_{free}	0.205 , 0.259 0.203 , 0.255	Depositor DCC
R_{free} test set	4161 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	45515	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TPO, MLA, EDO, GOL, PTR, A1CZ9

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	0.65	3/2869 (0.1%)	1.11	15/3890 (0.4%)
1	B	0.66	3/2869 (0.1%)	1.11	13/3890 (0.3%)
1	C	0.64	1/2785 (0.0%)	1.14	13/3778 (0.3%)
1	D	0.65	2/2869 (0.1%)	1.11	13/3890 (0.3%)
2	E	0.62	1/2766 (0.0%)	1.11	8/3732 (0.2%)
2	F	0.60	0/2786	1.11	12/3759 (0.3%)
2	G	0.59	1/2740 (0.0%)	1.12	9/3695 (0.2%)
2	H	0.61	0/2712	1.11	10/3660 (0.3%)
All	All	0.63	11/22396 (0.0%)	1.12	93/30294 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	HIS	CG-CD2	5.45	1.41	1.35
1	D	199	HIS	CG-CD2	5.34	1.41	1.35
1	C	199	HIS	CG-CD2	5.33	1.41	1.35
1	A	64	HIS	CG-CD2	5.29	1.41	1.35
2	E	108	HIS	CG-CD2	5.26	1.41	1.35

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	126	ASN	CA-CB-CG	7.66	120.26	112.60
2	H	267	HIS	ND1-CE1-NE2	7.59	115.99	108.40
2	E	267	HIS	ND1-CE1-NE2	7.49	115.89	108.40
2	F	126	ASN	CA-CB-CG	7.36	119.96	112.60
2	H	126	ASN	CA-CB-CG	7.02	119.62	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	265	SER	Peptide

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	2845	2822	2817	1	0
1	B	2845	2823	2817	1	0
1	C	2734	2732	2729	2	1
1	D	2845	2822	2817	2	0
2	E	2710	2751	2743	1	0
2	F	2730	2770	2768	3	0
2	G	2688	2740	2734	3	1
2	H	2657	2698	2694	1	0
3	A	38	24	0	0	0
3	B	38	24	0	0	0
3	C	38	24	0	0	0
3	D	38	24	0	0	0
4	A	4	6	6	0	0
4	B	4	6	6	0	0
4	C	4	6	6	0	0
4	D	4	6	6	0	0
5	E	6	8	8	0	0
6	E	7	4	2	0	0
7	A	74	148	0	0	0
7	B	36	72	0	0	0
7	C	39	78	0	0	0
7	D	49	98	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	43	86	0	0	0
7	F	37	74	0	0	0
7	G	18	36	0	0	0
7	H	34	68	0	0	0
All	All	22565	22950	22153	12	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 0.

The worst 5 of 12 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:C:186:ARG:N	2:H:267:HIS:HD1	2.04	0.55
2:G:271:ILE:N	2:G:271:ILE:HD12	2.24	0.52
2:F:271:ILE:HD12	2:F:271:ILE:N	2.26	0.51
2:F:93:LYS:HD2	2:F:138:MET:HE1	1.96	0.48
2:G:271:ILE:HD12	2:G:271:ILE:H	1.78	0.48

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:C:263:TPO:O3P	2:G:96:GLN:HE21[2_445]	1.59	0.01

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	346/363 (95%)	328 (95%)	16 (5%)	2 (1%)	21 38
1	B	346/363 (95%)	328 (95%)	17 (5%)	1 (0%)	36 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	333/363 (92%)	313 (94%)	19 (6%)	1 (0%)	36 54
1	D	346/363 (95%)	329 (95%)	16 (5%)	1 (0%)	36 54
2	E	329/363 (91%)	317 (96%)	12 (4%)	0	100 100
2	F	332/363 (92%)	313 (94%)	17 (5%)	2 (1%)	21 38
2	G	324/363 (89%)	305 (94%)	19 (6%)	0	100 100
2	H	320/363 (88%)	303 (95%)	17 (5%)	0	100 100
All	All	2676/2904 (92%)	2536 (95%)	133 (5%)	7 (0%)	36 54

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	SER
1	B	168	ASP
1	D	168	ASP
1	A	326	SER
1	C	168	ASP

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	308/317 (97%)	305 (99%)	3 (1%)	68 83
1	B	308/317 (97%)	302 (98%)	6 (2%)	50 72
1	C	299/317 (94%)	298 (100%)	1 (0%)	86 93
1	D	308/317 (97%)	304 (99%)	4 (1%)	61 79
2	E	301/322 (94%)	296 (98%)	5 (2%)	53 75
2	F	303/322 (94%)	300 (99%)	3 (1%)	68 83
2	G	297/322 (92%)	293 (99%)	4 (1%)	61 79
2	H	296/322 (92%)	290 (98%)	6 (2%)	48 71
All	All	2420/2556 (95%)	2388 (99%)	32 (1%)	61 79

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	267	HIS
2	H	288	ASN
1	D	229	ILE
1	D	227	ASP
2	H	308	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	151	GLN
2	H	217	HIS
2	H	113	GLN
2	H	218	ASN
2	E	96	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 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	TPO	A	180	1	8,10,11	0.91	0	10,14,16	0.96	0
1	TPO	B	180	1	8,10,11	1.07	0	10,14,16	0.83	0
1	PTR	D	182	1	15,16,17	1.25	0	17,22,24	0.53	0
1	TPO	D	263	1	8,10,11	0.93	0	10,14,16	1.04	1 (10%)
1	PTR	A	182	1	15,16,17	1.23	0	17,22,24	0.55	0
1	TPO	C	263	1	8,10,11	1.12	1 (12%)	10,14,16	0.94	0
1	TPO	D	180	1	8,10,11	1.01	0	10,14,16	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PTR	B	182	1	15,16,17	1.16	0	17,22,24	0.83	1 (5%)
1	TPO	A	263	1	8,10,11	0.99	0	10,14,16	1.03	1 (10%)
1	TPO	B	263	1	8,10,11	1.04	1 (12%)	10,14,16	0.95	1 (10%)

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	TPO	A	180	1	-	1/9/11/13	-
1	TPO	B	180	1	-	2/9/11/13	-
1	PTR	D	182	1	-	1/10/11/13	0/1/1/1
1	TPO	D	263	1	-	0/9/11/13	-
1	PTR	A	182	1	-	2/10/11/13	0/1/1/1
1	TPO	C	263	1	-	2/9/11/13	-
1	TPO	D	180	1	-	1/9/11/13	-
1	PTR	B	182	1	-	1/10/11/13	0/1/1/1
1	TPO	A	263	1	-	1/9/11/13	-
1	TPO	B	263	1	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	TPO	P-OG1	2.09	1.63	1.59
1	B	263	TPO	P-OG1	2.04	1.63	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	263	TPO	P-OG1-CB	-2.18	117.40	123.33
1	B	263	TPO	P-OG1-CB	-2.10	117.61	123.33
1	B	182	PTR	O2P-P-OH	2.10	111.52	105.32
1	A	263	TPO	P-OG1-CB	-2.07	117.70	123.33

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	180	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	A	182	PTR	O-C-CA-CB
1	B	180	TPO	O-C-CA-CB
1	D	180	TPO	O-C-CA-CB
1	D	182	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	C	263	TPO	0	1

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
4	EDO	A	402	-	3,3,3	0.41	0	2,2,2	0.50	0
3	A1CZ9	D	401	-	38,43,43	1.44	7 (18%)	54,67,67	1.47	8 (14%)
3	A1CZ9	C	401	-	38,43,43	1.43	8 (21%)	54,67,67	1.48	9 (16%)
4	EDO	B	402	-	3,3,3	0.45	0	2,2,2	0.78	0
6	MLA	E	502	-	6,6,6	1.25	0	7,7,7	1.18	1 (14%)
3	A1CZ9	B	401	-	38,43,43	1.44	7 (18%)	54,67,67	1.46	9 (16%)
5	GOL	E	501	-	5,5,5	0.63	0	5,5,5	0.83	0
4	EDO	C	402	-	3,3,3	0.41	0	2,2,2	0.43	0
3	A1CZ9	A	401	-	38,43,43	1.40	7 (18%)	54,67,67	1.46	8 (14%)
4	EDO	D	402	-	3,3,3	0.42	0	2,2,2	0.74	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	A	402	-	-	0/1/1/1	-
3	A1CZ9	D	401	-	-	0/18/42/42	0/6/6/6
3	A1CZ9	C	401	-	-	2/18/42/42	0/6/6/6
4	EDO	B	402	-	-	1/1/1/1	-
6	MLA	E	502	-	-	2/4/4/4	-
3	A1CZ9	B	401	-	-	3/18/42/42	0/6/6/6
5	GOL	E	501	-	-	0/4/4/4	-
4	EDO	C	402	-	-	0/1/1/1	-
3	A1CZ9	A	401	-	-	3/18/42/42	0/6/6/6
4	EDO	D	402	-	-	0/1/1/1	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	A1CZ9	C15-C14	-3.48	1.43	1.48
3	C	401	A1CZ9	C15-C14	-3.41	1.43	1.48
3	B	401	A1CZ9	C15-C14	-3.31	1.43	1.48
3	A	401	A1CZ9	C15-C14	-3.20	1.43	1.48
3	C	401	A1CZ9	C17-C18	3.05	1.44	1.38

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	A1CZ9	O3-C14-N4	4.35	128.88	125.58
3	A	401	A1CZ9	O3-C14-N4	4.27	128.81	125.58
3	D	401	A1CZ9	O3-C14-N4	4.22	128.78	125.58
3	B	401	A1CZ9	O3-C14-N4	4.20	128.76	125.58
3	D	401	A1CZ9	C25-C26-C27	3.15	120.03	116.67

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	A1CZ9	C2-C3-N4-C21
6	E	502	MLA	C1-C2-C3-O3B
3	B	401	A1CZ9	C4-C3-N4-C14
6	E	502	MLA	C1-C2-C3-O3A

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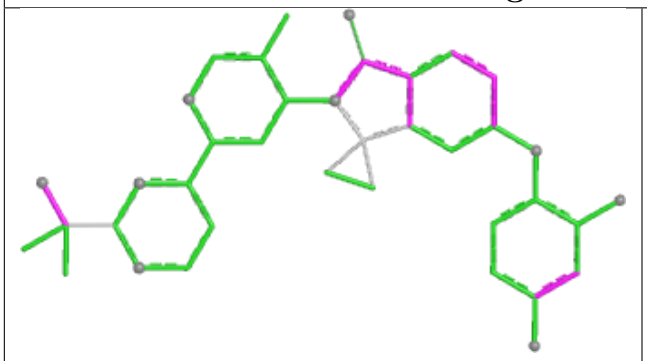
Mol	Chain	Res	Type	Atoms
3	B	401	A1CZ9	C4-C3-N4-C21

There are no ring outliers.

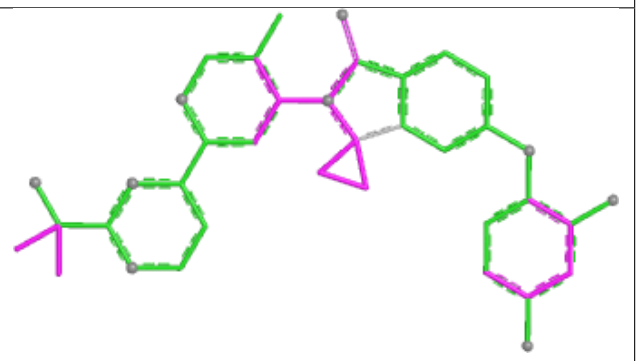
No monomer is involved in short contacts.

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 then 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.

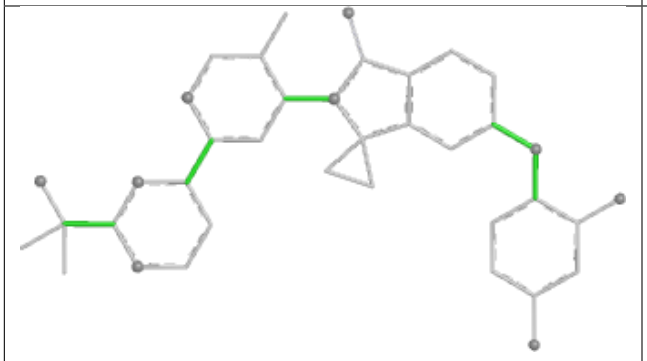
Ligand A1CZ9 D 401



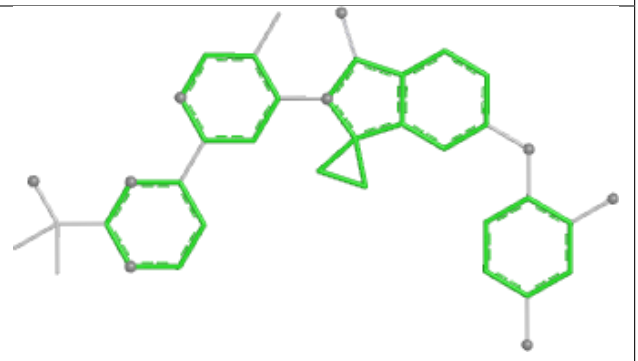
Bond lengths



Bond angles

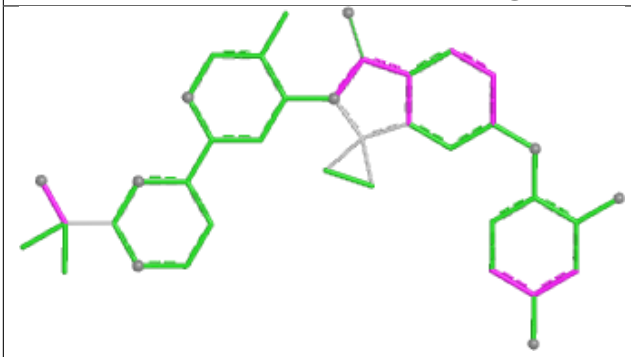


Torsions

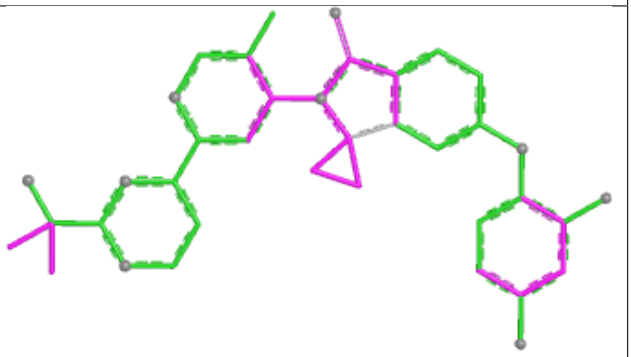


Rings

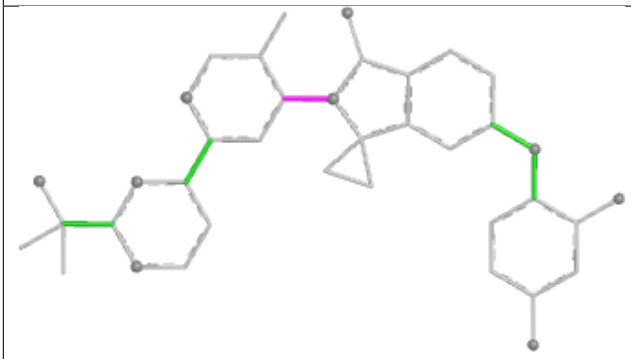
Ligand A1CZ9 C 401



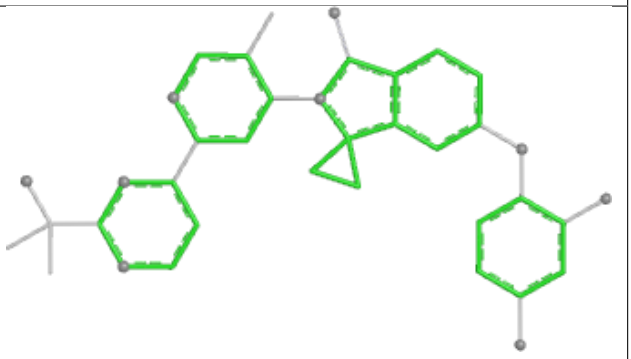
Bond lengths



Bond angles

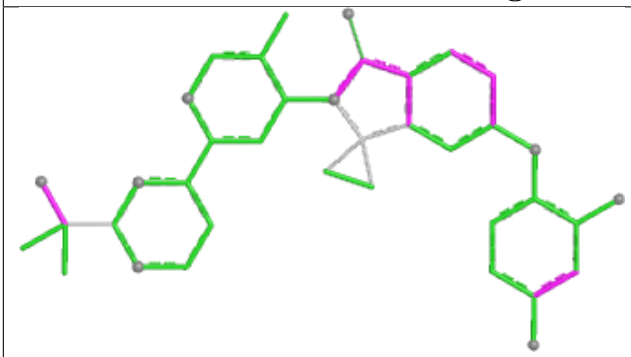


Torsions

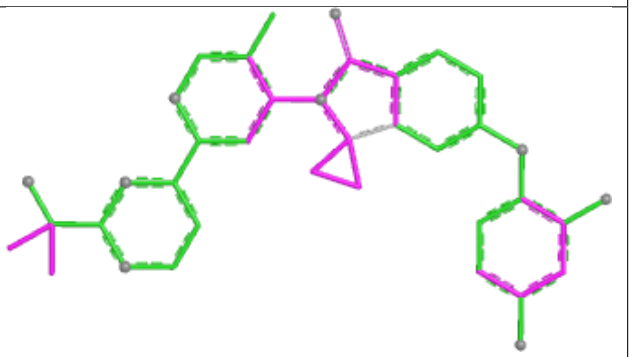


Rings

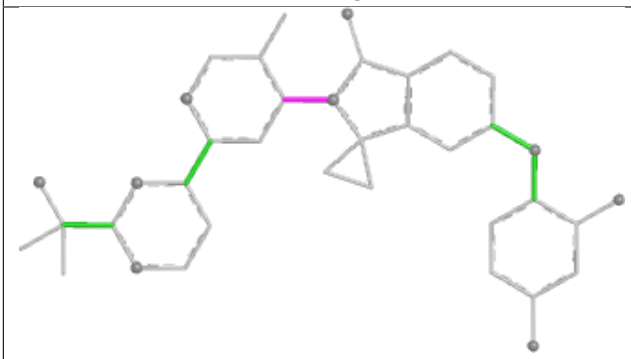
Ligand A1CZ9 B 401



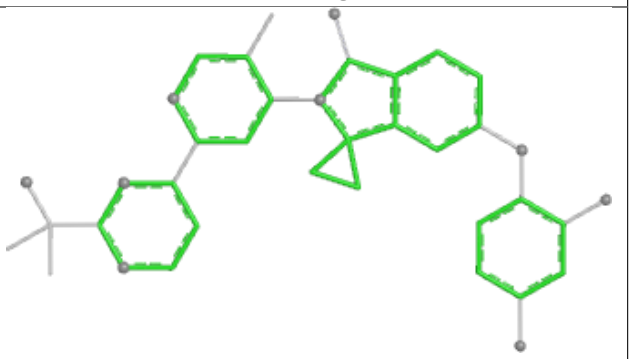
Bond lengths



Bond angles

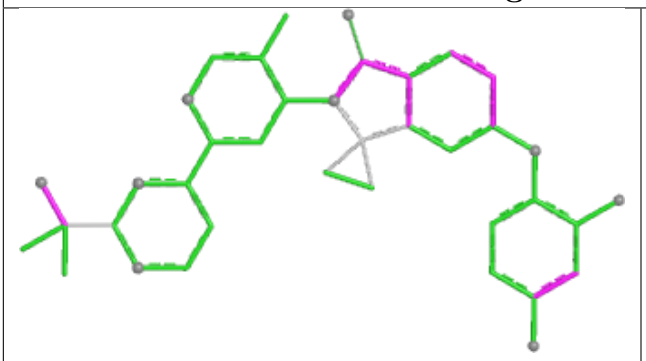


Torsions

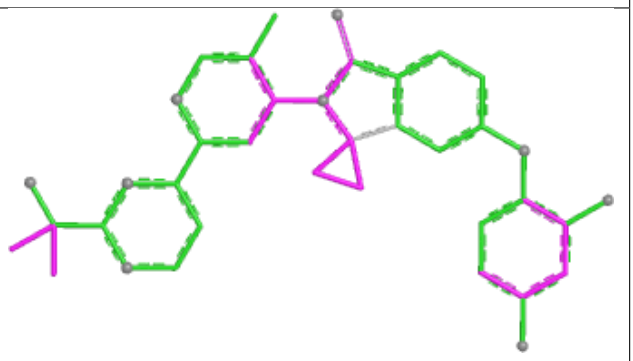


Rings

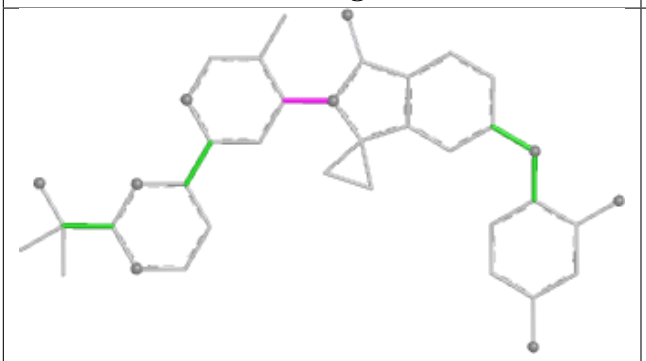
Ligand A1CZ9 A 401



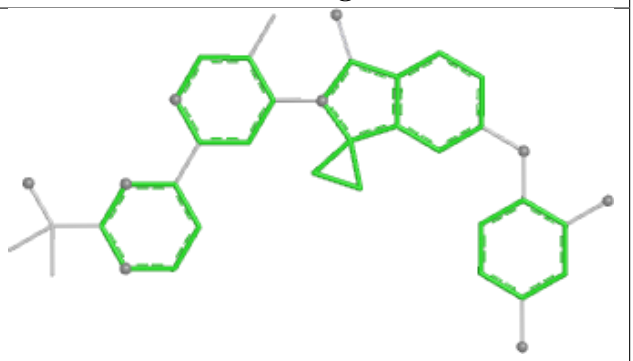
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	348/363 (95%)	-0.36	2 (0%) 85 82	10, 31, 65, 113	0
1	B	348/363 (95%)	0.19	19 (5%) 30 23	17, 47, 101, 118	0
1	C	337/363 (92%)	0.02	14 (4%) 40 32	17, 44, 81, 116	0
1	D	348/363 (95%)	-0.18	3 (0%) 81 76	16, 40, 77, 99	0
2	E	333/363 (91%)	0.01	12 (3%) 46 36	17, 41, 88, 122	0
2	F	336/363 (92%)	0.20	17 (5%) 33 26	19, 48, 103, 136	0
2	G	332/363 (91%)	0.28	18 (5%) 31 23	20, 52, 101, 127	0
2	H	326/363 (89%)	0.50	22 (6%) 24 17	19, 59, 104, 117	0
All	All	2708/2904 (93%)	0.08	107 (3%) 42 33	10, 45, 95, 136	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	268	GLY	5.3
2	H	158	PHE	4.6
2	H	267	HIS	4.4
2	E	282	GLY	4.4
2	H	396	ALA	4.2

6.2 Non-standard residues in protein, DNA, RNA chains

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^{th} 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	TPO	C	263	11/12	0.79	0.14	48,72,124,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	B	180	11/12	0.80	0.14	91,97,101,102	0
1	PTR	B	182	16/17	0.86	0.14	84,99,110,117	0
1	TPO	D	263	11/12	0.86	0.13	48,72,116,116	0
1	PTR	D	182	16/17	0.89	0.13	48,53,72,80	0
1	TPO	B	263	11/12	0.90	0.13	36,53,93,97	0
1	PTR	A	182	16/17	0.90	0.10	30,46,77,79	0
1	TPO	D	180	11/12	0.91	0.10	44,51,64,64	0
1	TPO	A	263	11/12	0.94	0.10	26,52,87,87	0
1	TPO	A	180	11/12	0.97	0.06	22,29,45,47	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

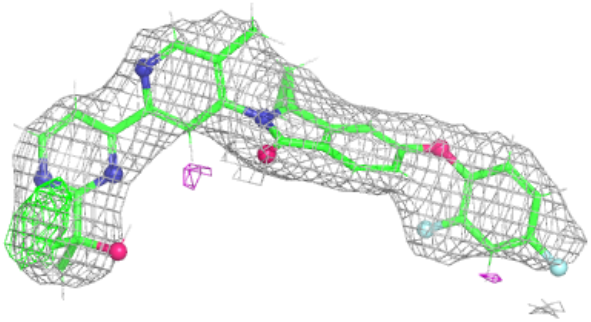
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

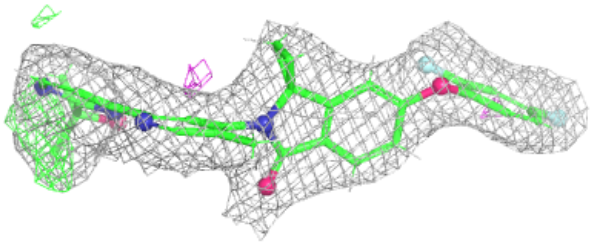
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	402	4/4	0.79	0.21	66,75,77,77	0
5	GOL	E	501	6/6	0.83	0.15	46,50,55,56	0
4	EDO	C	402	4/4	0.86	0.15	45,49,52,54	0
4	EDO	A	402	4/4	0.88	0.14	30,46,54,54	0
4	EDO	D	402	4/4	0.90	0.12	54,57,59,59	0
6	MLA	E	502	7/7	0.90	0.15	35,59,63,73	0
3	A1CZ9	B	401	38/38	0.93	0.11	27,35,52,63	0
3	A1CZ9	D	401	38/38	0.94	0.10	23,32,50,54	0
3	A1CZ9	C	401	38/38	0.96	0.08	17,28,49,50	0
3	A1CZ9	A	401	38/38	0.96	0.08	14,23,45,46	0

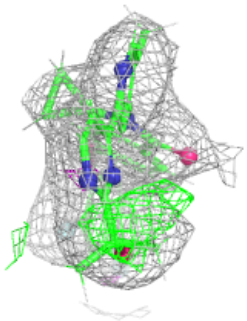
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CZ9 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)

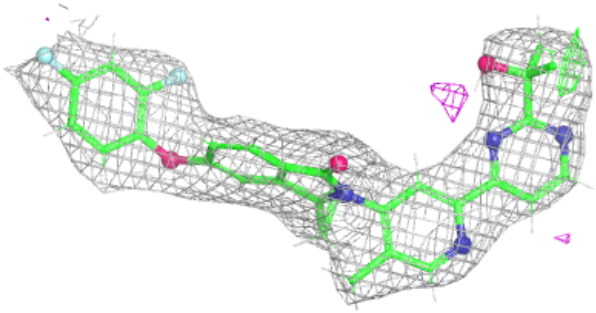


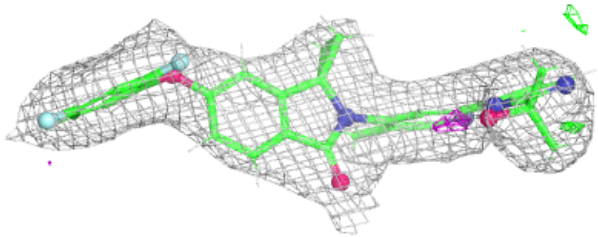


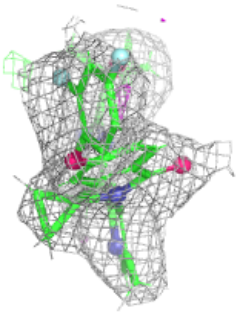


Electron density around A1CZ9 D 401:

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

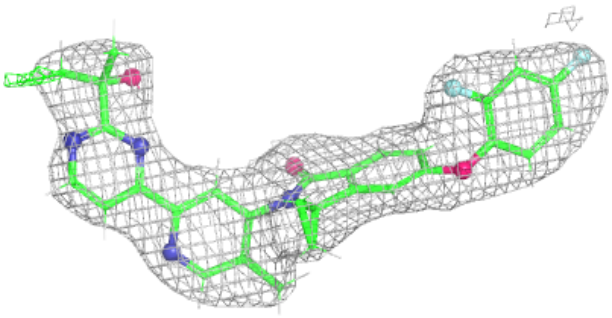




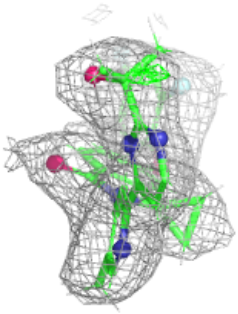


Electron density around A1CZ9 C 401:

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

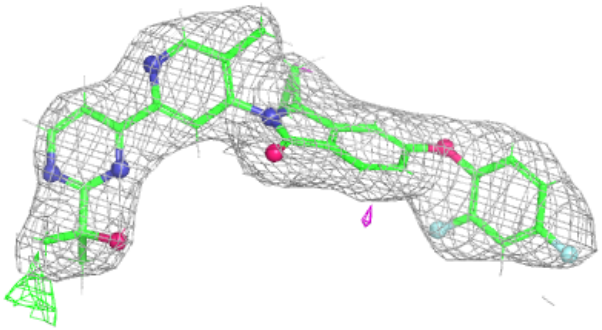


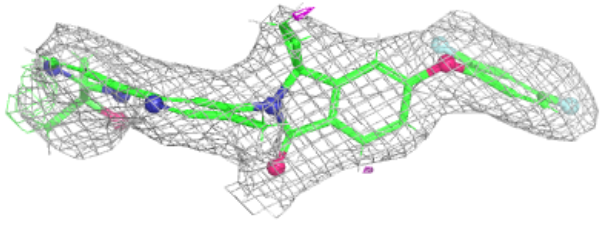


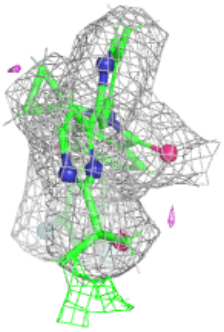


Electron density around A1CZ9 A 401:

$2mF_o$-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 (i)

There are no such residues in this entry.