wwPDB X-ray Structure Validation Summary Report (i)

Nov 2, 2026 – 08:10 AM EST

PDB ID	:	9Z3N / pdb_00009z3n
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:

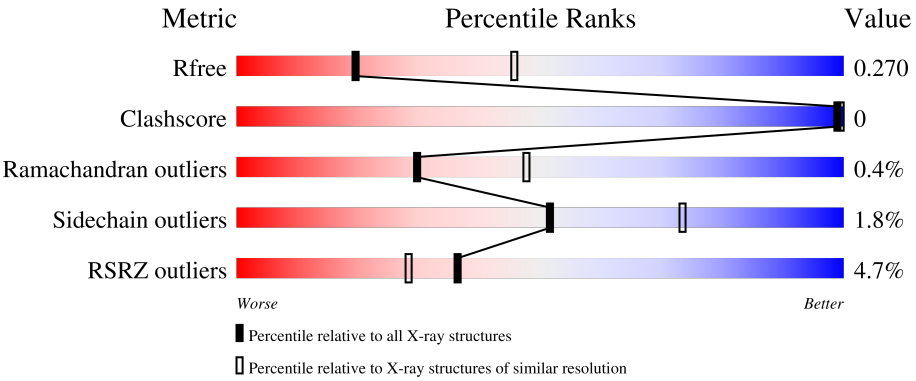
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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.



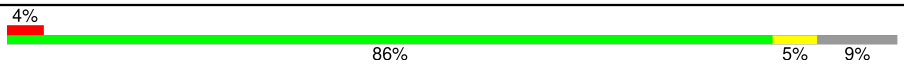
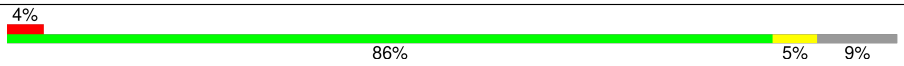
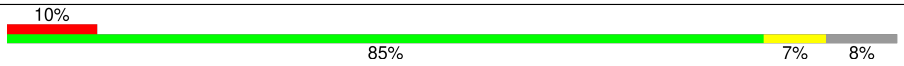
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	2% 89% 7% ·
1	B	363	5% 91% 6% ·
1	C	363	5% 91% 6% ·
1	D	363	2% 90% 7% ·
2	E	363	4% 86% 5% 9%

Continued on next page...

Continued from previous page...

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 44797 atoms, of which 22427 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
			5666	1813	2821	483	533	3	13			
1	C	353	Total	C	H	N	O	P	S	0	0	0
			5693	1821	2833	486	537	3	13			
1	D	350	Total	C	H	N	O	P	S	0	0	0
			5655	1809	2818	482	530	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	331	Total	C	H	N	O	S	0	0	0
			5423	1713	2730	464	498	18			
2	F	330	Total	C	H	N	O	S	0	0	0
			5400	1707	2720	460	494	19			

Continued on next page...

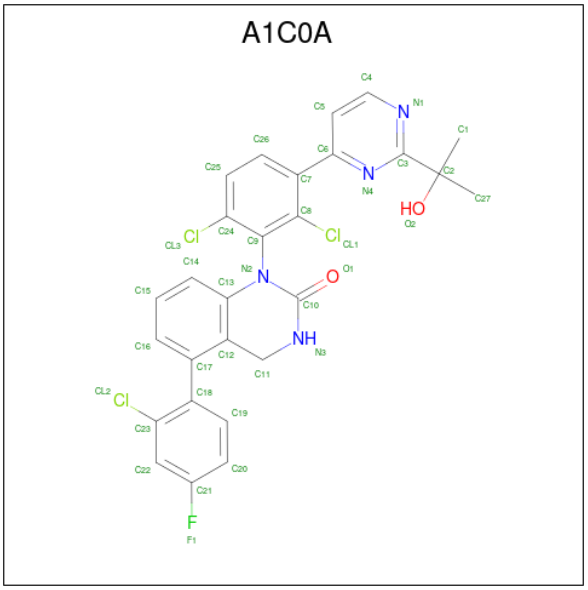
Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	330	Total	C	H	N	O	S	0	0	0
			5411	1709	2731	460	492	19			
2	H	333	Total	C	H	N	O	S	0	0	0
			5453	1724	2746	467	497	19			

There are 12 discrepancies between the modelled and reference sequences:

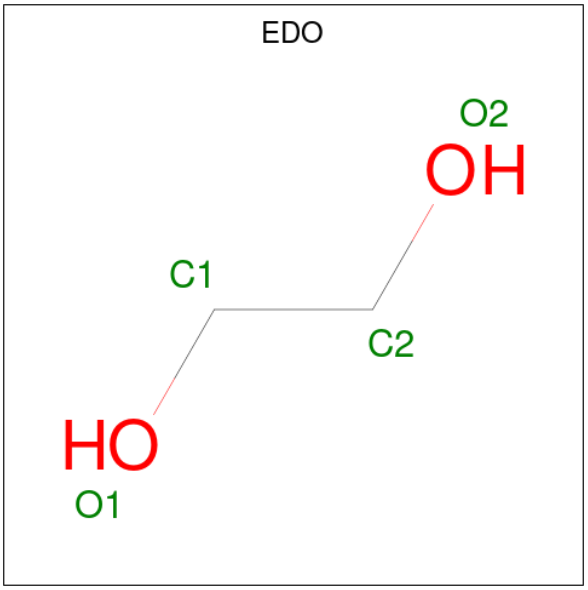
Chain	Residue	Modelled	Actual	Comment	Reference
E	38	GLY	-	expression tag	UNP P49137
E	39	GLY	-	expression tag	UNP P49137
E	40	GLY	-	expression tag	UNP P49137
F	38	GLY	-	expression tag	UNP P49137
F	39	GLY	-	expression tag	UNP P49137
F	40	GLY	-	expression tag	UNP P49137
G	38	GLY	-	expression tag	UNP P49137
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 (1M,5P)-5-(2-chloro-4-fluorophenyl)-1-{(3P)-2,6-dichloro-3-[2-(2-hydroxypropan-2-yl)pyrimidin-4-yl]phenyl}quinazolin-2(1H)-one (CCD ID: A1C0A) (formula: $C_{27}H_{20}Cl_3FN_4O_2$) (labeled as "Ligand of Interest" by depositor).



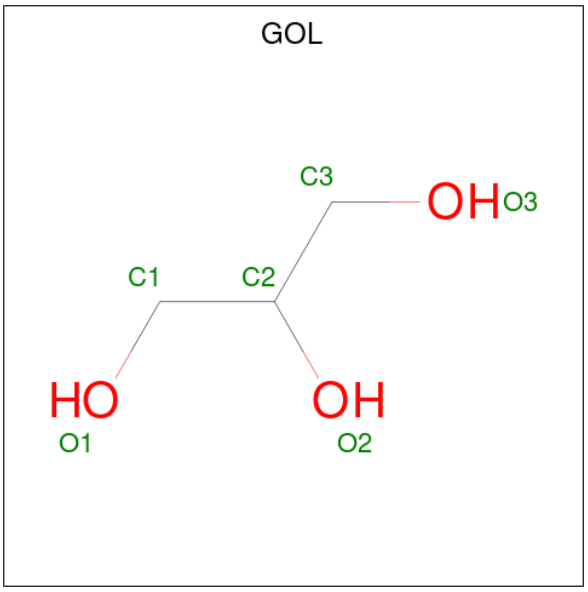
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	H	N	O	0	0
			57	27	3	1	20	4	2		
3	B	1	Total	C	Cl	F	H	N	O	0	0
			57	27	3	1	20	4	2		
3	C	1	Total	C	Cl	F	H	N	O	0	0
			57	27	3	1	20	4	2		
3	D	1	Total	C	Cl	F	H	N	O	0	0
			57	27	3	1	20	4	2		

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



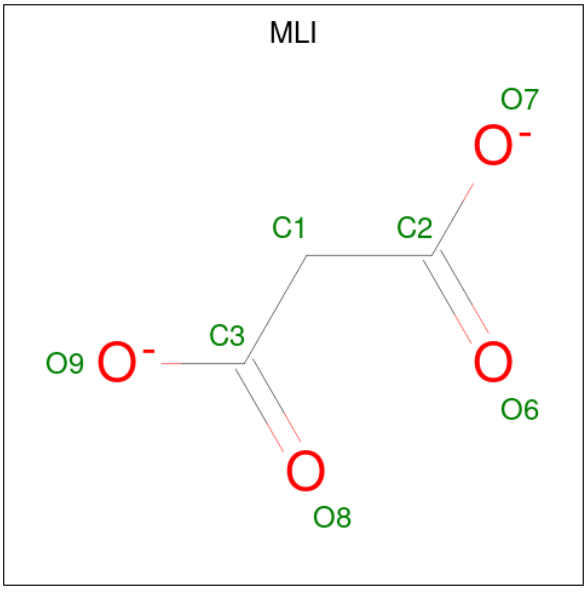
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		

- 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 MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 7 is water.

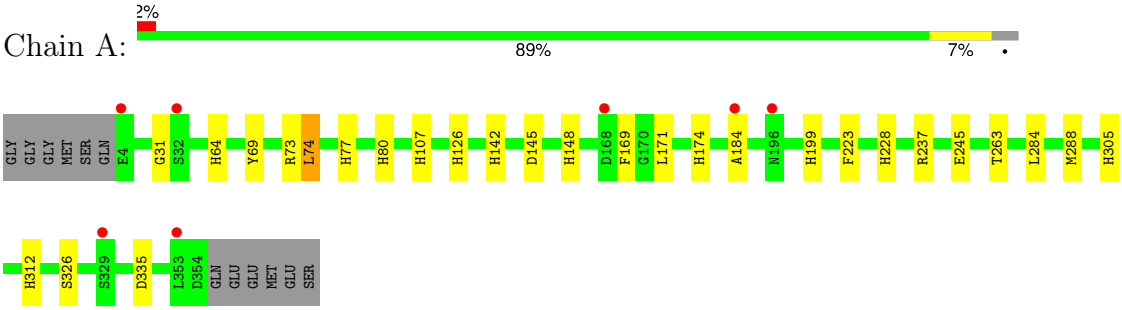
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	13	Total H O 39 26 13	0	0
7	B	5	Total H O 15 10 5	0	0
7	C	1	Total H O 3 2 1	0	0
7	D	8	Total H O 24 16 8	0	0
7	E	4	Total H O 12 8 4	0	0
7	F	7	Total H O 21 14 7	0	0
7	G	4	Total H O 12 8 4	0	0
7	H	4	Total H O 12 8 4	0	0

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.

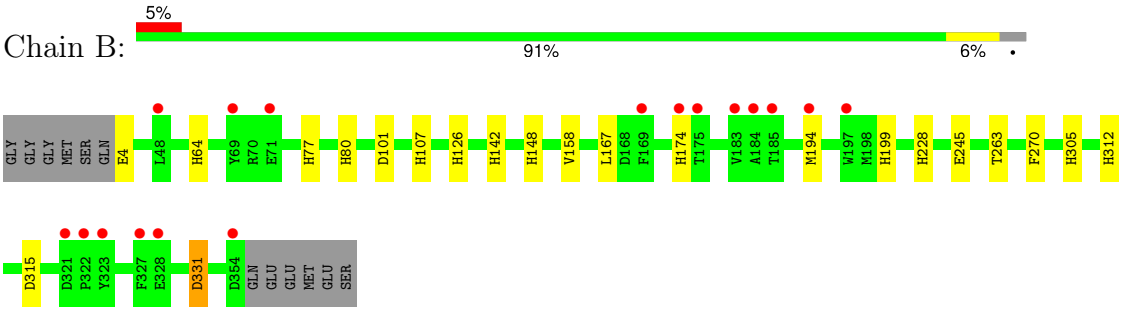
• Molecule 1: Mitogen-activated protein kinase 14

Chain A:



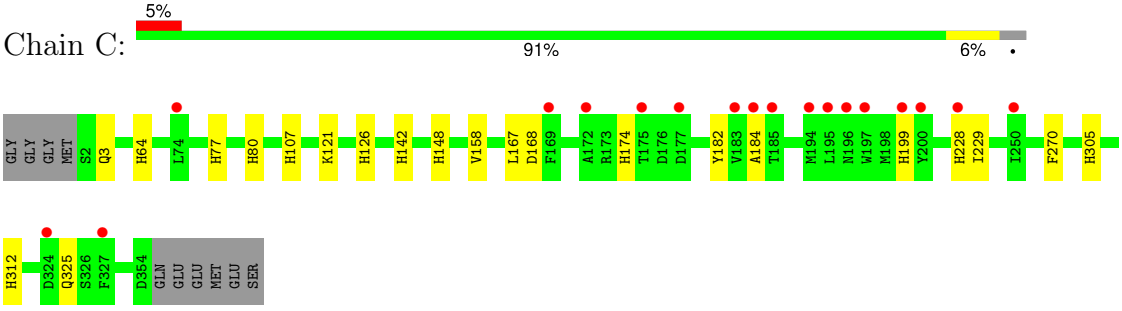
• Molecule 1: Mitogen-activated protein kinase 14

Chain B:



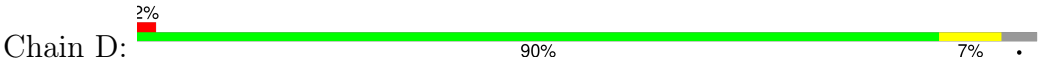
• Molecule 1: Mitogen-activated protein kinase 14

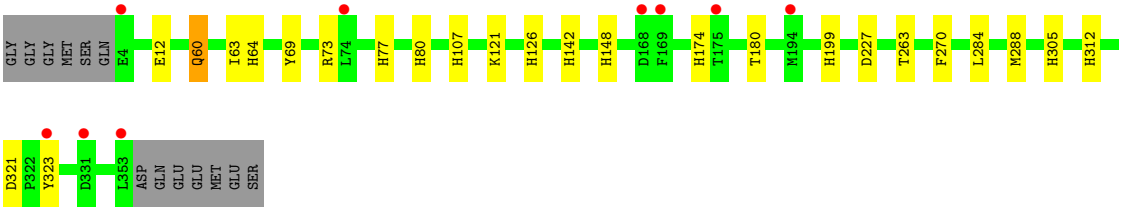
Chain C:



• Molecule 1: Mitogen-activated protein kinase 14

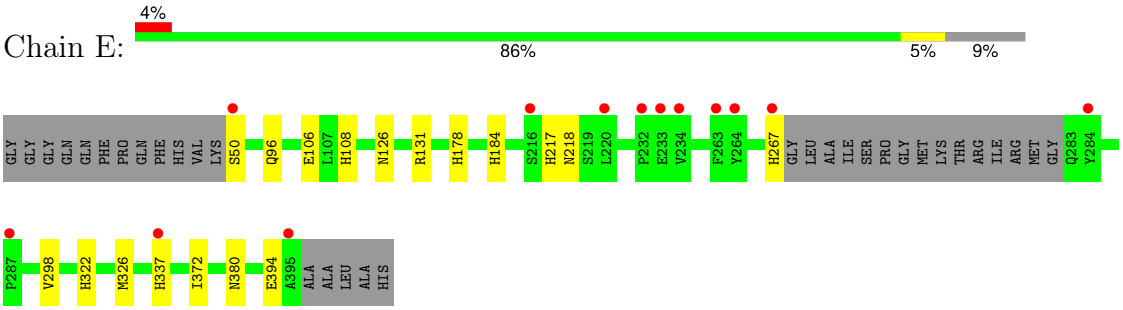
Chain D:





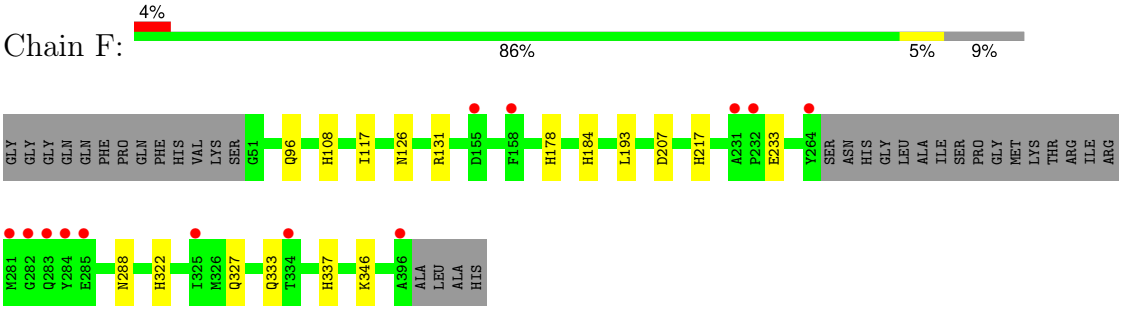
• Molecule 2: MAP kinase-activated protein kinase 2

Chain E:



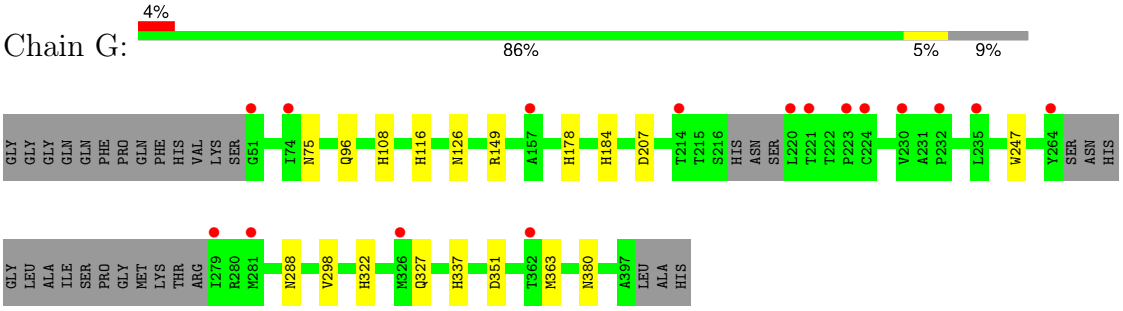
• Molecule 2: MAP kinase-activated protein kinase 2

Chain F:



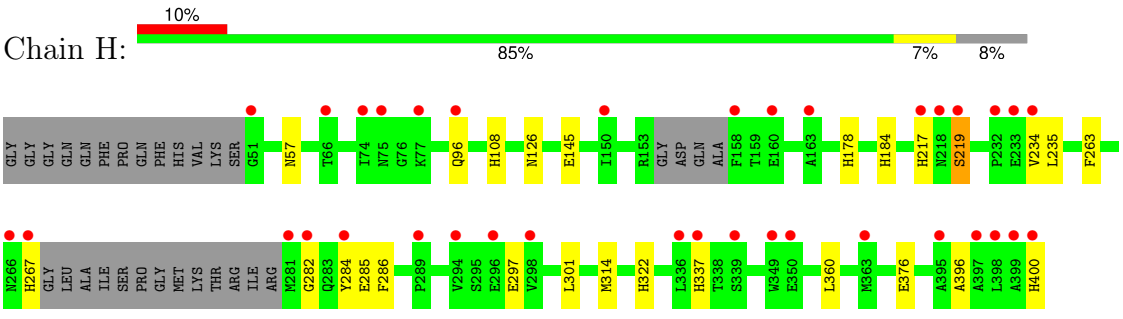
• Molecule 2: MAP kinase-activated protein kinase 2

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	63.41Å 229.83Å 126.55Å 90.00° 103.75° 90.00°	Depositor
Resolution (Å)	48.70 – 2.85 48.70 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.70-2.85) 99.9 (48.70-2.85)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.86Å)	Xtriage
Refinement program	PRIME-X	Depositor
R, R_{free}	0.228 , 0.272 0.228 , 0.270	Depositor DCC
R_{free} test set	4120 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	44797	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.77% 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: EDO, A1C0A, TPO, GOL, PTR, MLI

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%)	1.10	13/3890 (0.3%)
1	B	0.65	2/2869 (0.1%)	1.11	13/3890 (0.3%)
1	C	0.64	1/2884 (0.0%)	1.11	13/3910 (0.3%)
1	D	0.64	1/2861 (0.0%)	1.13	14/3879 (0.4%)
2	E	0.62	1/2749 (0.0%)	1.11	8/3711 (0.2%)
2	F	0.60	0/2735	1.10	9/3691 (0.2%)
2	G	0.59	1/2733 (0.0%)	1.13	10/3686 (0.3%)
2	H	0.62	0/2763	1.14	11/3727 (0.3%)
All	All	0.63	9/22463 (0.0%)	1.12	91/30384 (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 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	116	HIS	CG-CD2	5.45	1.41	1.35
2	E	108	HIS	CG-CD2	5.38	1.41	1.35
1	C	174	HIS	CG-CD2	5.38	1.41	1.35
1	A	199	HIS	CG-CD2	5.28	1.41	1.35
1	A	64	HIS	CG-CD2	5.26	1.41	1.35

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	267	HIS	ND1-CE1-NE2	7.77	116.17	108.40
2	H	267	HIS	ND1-CE1-NE2	7.76	116.16	108.40
2	G	126	ASN	CA-CB-CG	7.70	120.30	112.60
2	H	126	ASN	CA-CB-CG	7.31	119.91	112.60
2	E	126	ASN	CA-CB-CG	7.24	119.84	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	233	GLU	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	3	0
1	B	2845	2821	2817	1	0
1	C	2860	2833	2830	2	0
1	D	2837	2818	2813	4	0
2	E	2693	2730	2723	1	0
2	F	2680	2720	2717	1	0
2	G	2680	2731	2727	1	0
2	H	2707	2746	2742	3	0
3	A	37	20	0	1	0
3	B	37	20	0	2	0
3	C	37	20	0	2	0
3	D	37	20	0	1	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	2	2	0	0
7	A	13	26	0	0	0
7	B	5	10	0	0	0
7	C	1	2	0	0	0
7	D	8	16	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	4	8	0	0	0
7	F	7	14	0	0	0
7	G	4	8	0	0	0
7	H	4	8	0	0	0
All	All	22370	22427	22220	19	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 19 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:D:63:ILE:HD12	1:D:63:ILE:H	1.70	0.56
2:F:96:GLN:HE22	2:F:131:ARG:HB3	1.72	0.54
1:A:284:LEU:HG	1:A:288:MET:HE2	1.90	0.53
1:D:284:LEU:HG	1:D:288:MET:HE2	1.91	0.53
1:D:69:TYR:CZ	1:D:73:ARG:HD2	2.45	0.51

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	346/363 (95%)	327 (94%)	16 (5%)	3 (1%)	14 28
1	B	346/363 (95%)	329 (95%)	17 (5%)	0	100 100
1	C	348/363 (96%)	329 (94%)	17 (5%)	2 (1%)	21 38
1	D	345/363 (95%)	330 (96%)	15 (4%)	0	100 100
2	E	327/363 (90%)	311 (95%)	15 (5%)	1 (0%)	36 54
2	F	326/363 (90%)	309 (95%)	16 (5%)	1 (0%)	36 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	G	324/363 (89%)	307 (95%)	16 (5%)	1 (0%)	36 54
2	H	327/363 (90%)	301 (92%)	24 (7%)	2 (1%)	21 38
All	All	2689/2904 (93%)	2543 (95%)	136 (5%)	10 (0%)	30 48

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	396	ALA
1	A	31	GLY
1	A	184	ALA
2	H	219	SER
1	A	326	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	308/317 (97%)	304 (99%)	4 (1%)	61 79
1	B	308/317 (97%)	302 (98%)	6 (2%)	50 72
1	C	310/317 (98%)	306 (99%)	4 (1%)	61 79
1	D	307/317 (97%)	303 (99%)	4 (1%)	61 79
2	E	300/322 (93%)	294 (98%)	6 (2%)	48 71
2	F	297/322 (92%)	293 (99%)	4 (1%)	61 79
2	G	296/322 (92%)	291 (98%)	5 (2%)	53 75
2	H	300/322 (93%)	289 (96%)	11 (4%)	30 55
All	All	2426/2556 (95%)	2382 (98%)	44 (2%)	51 73

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	75	ASN
2	H	219	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	96	GLN
2	G	327	GLN
2	H	235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	200	ASN
2	H	175	GLN
2	G	151	GLN
2	H	113	GLN
2	F	181	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

12 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	0.97	0	10,14,16	1.00	0
1	PTR	C	182	1	15,16,17	1.22	1 (6%)	17,22,24	1.12	1 (5%)
1	TPO	B	263	1	8,10,11	1.00	0	10,14,16	0.89	1 (10%)
1	PTR	A	182	1	15,16,17	1.14	0	17,22,24	0.68	0
1	TPO	D	263	1	8,10,11	1.17	1 (12%)	10,14,16	0.97	0
1	TPO	A	263	1	8,10,11	0.91	0	10,14,16	1.06	1 (10%)
1	TPO	D	180	1	8,10,11	0.95	0	10,14,16	1.03	1 (10%)
1	PTR	D	182	1	15,16,17	1.18	0	17,22,24	0.47	0
1	TPO	C	180	1	8,10,11	0.95	0	10,14,16	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	TPO	C	263	1	8,10,11	1.04	0	10,14,16	1.01	0
1	PTR	B	182	1	15,16,17	1.21	0	17,22,24	0.58	0
1	TPO	B	180	1	8,10,11	1.08	0	10,14,16	0.94	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
1	TPO	A	180	1	-	1/9/11/13	-
1	PTR	C	182	1	-	0/10/11/13	0/1/1/1
1	TPO	B	263	1	-	1/9/11/13	-
1	PTR	A	182	1	-	0/10/11/13	0/1/1/1
1	TPO	D	263	1	-	0/9/11/13	-
1	TPO	A	263	1	-	0/9/11/13	-
1	TPO	D	180	1	-	1/9/11/13	-
1	PTR	D	182	1	-	3/10/11/13	0/1/1/1
1	TPO	C	180	1	-	1/9/11/13	-
1	TPO	C	263	1	-	0/9/11/13	-
1	PTR	B	182	1	-	3/10/11/13	0/1/1/1
1	TPO	B	180	1	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	263	TPO	P-OG1	2.31	1.63	1.59
1	C	182	PTR	P-OH	2.24	1.63	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	263	TPO	P-OG1-CB	-2.29	117.11	123.33
1	C	182	PTR	OH-P-O1P	-2.23	102.03	109.48
1	B	263	TPO	P-OG1-CB	-2.06	117.72	123.33
1	D	180	TPO	P-OG1-CB	-2.04	117.77	123.33

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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	$\#\|Z\| > 2$
3	A1C0A	C	401	-	39,41,41	1.36	2 (5%)	52,62,62	1.21	5 (9%)
4	EDO	B	402	-	3,3,3	0.45	0	2,2,2	0.30	0
4	EDO	C	402	-	3,3,3	0.41	0	2,2,2	0.78	0
4	EDO	A	402	-	3,3,3	0.41	0	2,2,2	0.63	0
3	A1C0A	D	401	-	39,41,41	1.31	2 (5%)	52,62,62	1.15	4 (7%)
5	GOL	E	501	-	5,5,5	0.51	0	5,5,5	0.39	0
3	A1C0A	B	401	-	39,41,41	1.33	2 (5%)	52,62,62	1.20	5 (9%)
6	MLI	E	502	-	6,6,6	1.75	2 (33%)	7,7,7	1.06	0
4	EDO	D	402	-	3,3,3	0.40	0	2,2,2	0.75	0
3	A1C0A	A	401	-	39,41,41	1.30	2 (5%)	52,62,62	1.18	5 (9%)

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	A1C0A	C	401	-	-	0/18/31/31	0/5/5/5
4	EDO	B	402	-	-	0/1/1/1	-
4	EDO	C	402	-	-	0/1/1/1	-
4	EDO	A	402	-	-	0/1/1/1	-
3	A1C0A	D	401	-	-	0/18/31/31	0/5/5/5
5	GOL	E	501	-	-	0/4/4/4	-
3	A1C0A	B	401	-	-	0/18/31/31	0/5/5/5
6	MLI	E	502	-	-	0/4/4/4	-
4	EDO	D	402	-	-	1/1/1/1	-
3	A1C0A	A	401	-	-	0/18/31/31	0/5/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	A1C0A	C7-C8	4.95	1.45	1.39
3	B	401	A1C0A	C7-C8	4.75	1.44	1.39
3	D	401	A1C0A	C7-C8	4.66	1.44	1.39
3	A	401	A1C0A	C7-C8	4.63	1.44	1.39
6	E	502	MLI	C1-C3	2.43	1.54	1.51

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	A1C0A	C9-N2-C10	3.24	120.69	115.42
3	C	401	A1C0A	C9-N2-C10	3.01	120.31	115.42
3	A	401	A1C0A	C9-N2-C10	2.93	120.19	115.42
3	D	401	A1C0A	C9-N2-C10	2.89	120.12	115.42
3	C	401	A1C0A	C24-C9-N2	-2.88	119.22	121.18

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	402	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	A1C0A	2	0

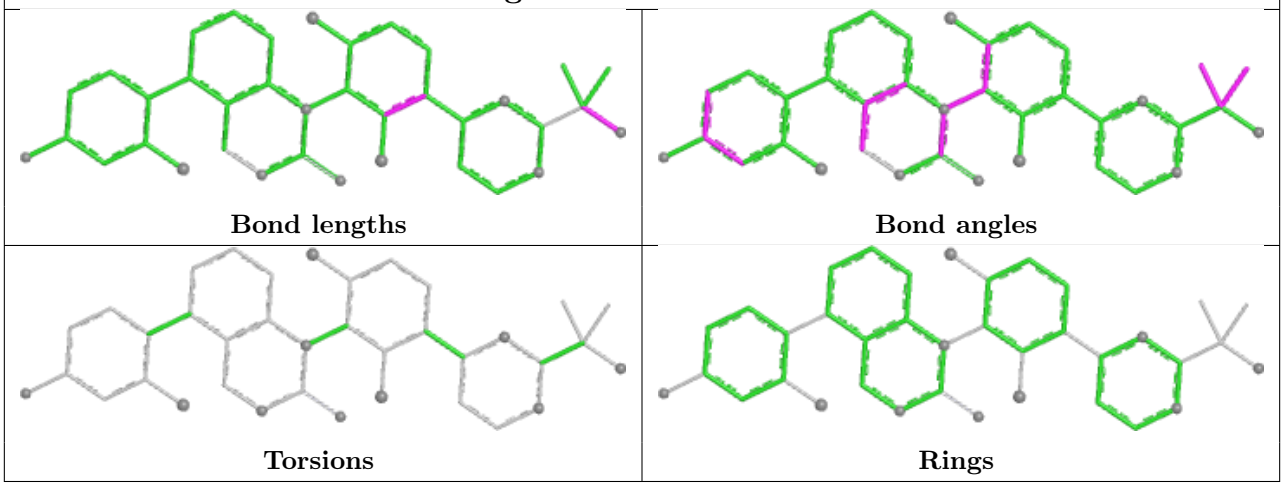
Continued on next page...

Continued from previous page...

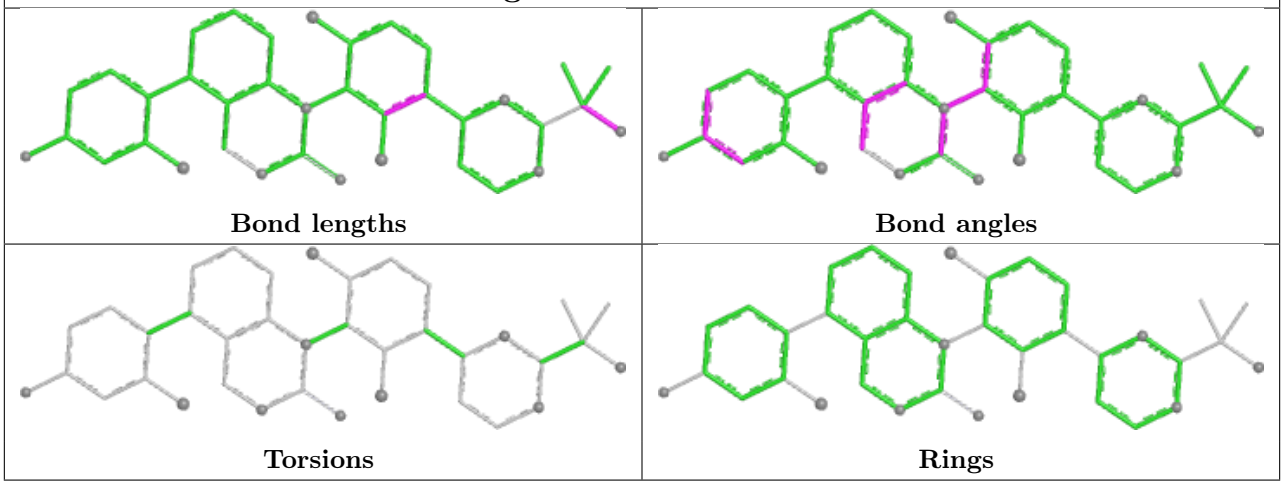
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	A1C0A	1	0
3	B	401	A1C0A	2	0
3	A	401	A1C0A	1	0

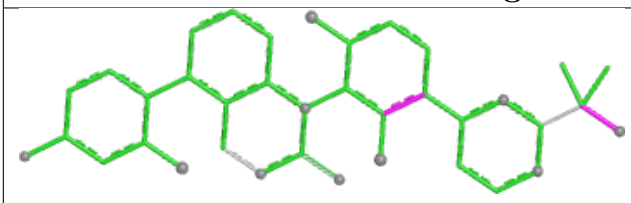
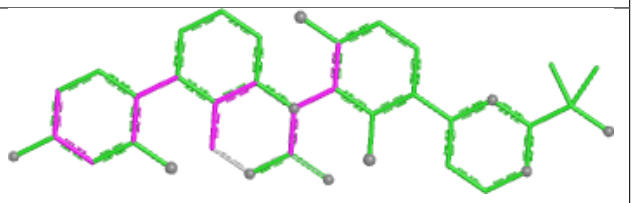
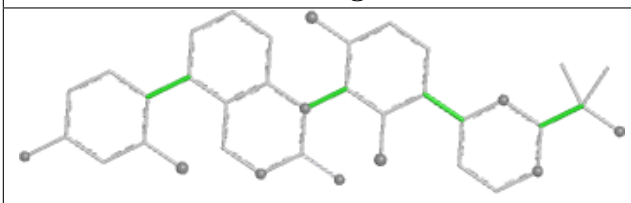
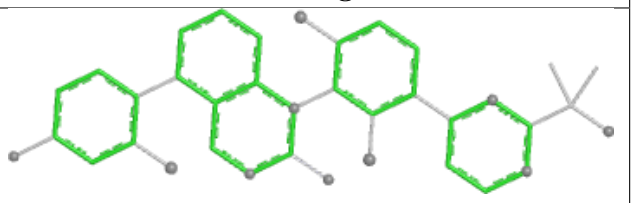
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

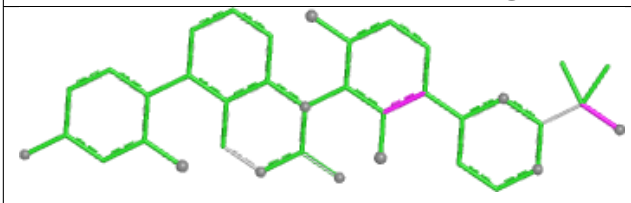
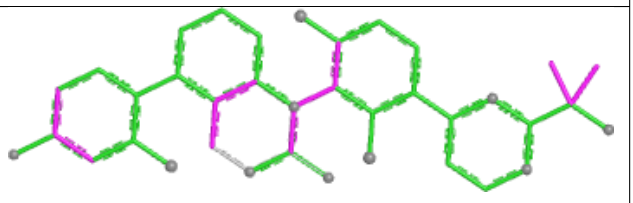
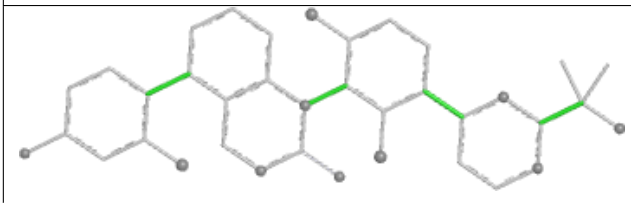
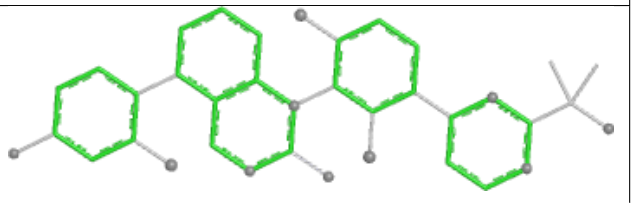
Ligand A1C0A C 401



Ligand A1C0A D 401



Ligand A1C0A B 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1C0A 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%)	-0.05	7 (2%) 65 57	21, 43, 80, 106	0
1	B	348/363 (95%)	0.36	17 (4%) 35 27	26, 56, 107, 134	0
1	C	350/363 (96%)	0.35	18 (5%) 33 26	29, 57, 103, 134	0
1	D	347/363 (95%)	0.02	9 (2%) 57 48	16, 48, 86, 105	0
2	E	331/363 (91%)	0.29	13 (3%) 43 34	25, 58, 97, 123	0
2	F	330/363 (90%)	0.37	13 (3%) 43 34	28, 59, 107, 126	1 (0%)
2	G	330/363 (90%)	0.46	16 (4%) 35 28	28, 66, 107, 127	0
2	H	333/363 (91%)	0.70	36 (10%) 11 8	32, 70, 118, 142	1 (0%)
All	All	2717/2904 (93%)	0.31	129 (4%) 36 28	16, 57, 106, 142	2 (0%)

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	158	PHE	5.1
1	C	169	PHE	4.5
1	B	184	ALA	4.3
2	E	267	HIS	4.1
1	C	194	MET	4.0

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	PTR	C	182	16/17	0.44	0.21	128,136,156,158	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	B	180	11/12	0.69	0.17	85,94,102,103	0
1	TPO	C	180	11/12	0.72	0.17	120,125,130,131	0
1	PTR	B	182	16/17	0.76	0.18	94,100,105,109	0
1	TPO	D	263	11/12	0.84	0.14	54,67,105,109	0
1	PTR	A	182	16/17	0.86	0.11	54,68,97,99	0
1	TPO	C	263	11/12	0.87	0.11	69,86,115,115	0
1	TPO	A	263	11/12	0.91	0.10	44,50,88,90	0
1	PTR	D	182	16/17	0.91	0.11	48,60,68,72	0
1	TPO	B	263	11/12	0.91	0.11	39,57,108,109	0
1	TPO	A	180	11/12	0.95	0.07	26,46,55,64	0
1	TPO	D	180	11/12	0.95	0.07	49,54,62,62	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

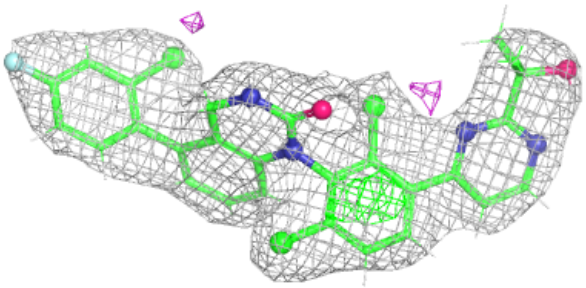
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

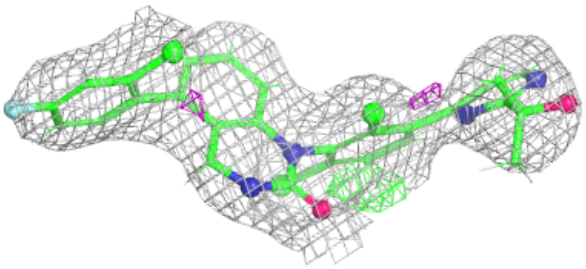
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	C	402	4/4	0.79	0.20	64,68,70,71	0
5	GOL	E	501	6/6	0.79	0.20	62,67,78,80	0
4	EDO	B	402	4/4	0.81	0.15	51,53,56,58	0
4	EDO	D	402	4/4	0.84	0.15	71,73,79,81	0
4	EDO	A	402	4/4	0.87	0.19	66,73,78,80	0
6	MLI	E	502	7/7	0.91	0.15	87,93,98,99	0
3	A1C0A	C	401	37/37	0.92	0.11	26,44,53,65	0
3	A1C0A	D	401	37/37	0.93	0.10	17,42,51,64	0
3	A1C0A	A	401	37/37	0.94	0.08	14,29,45,61	0
3	A1C0A	B	401	37/37	0.94	0.09	29,40,58,73	0

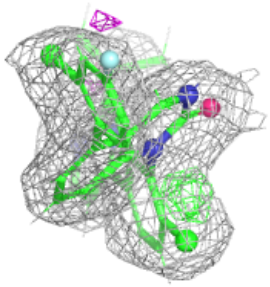
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1C0A 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)

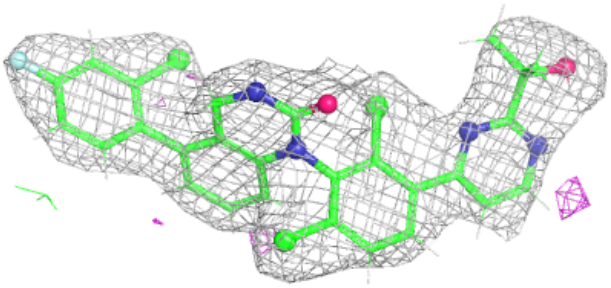


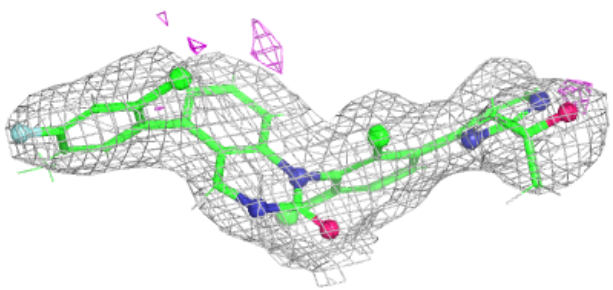


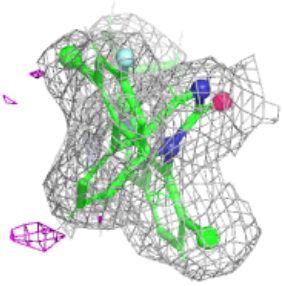


Electron density around A1C0A D 401:

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

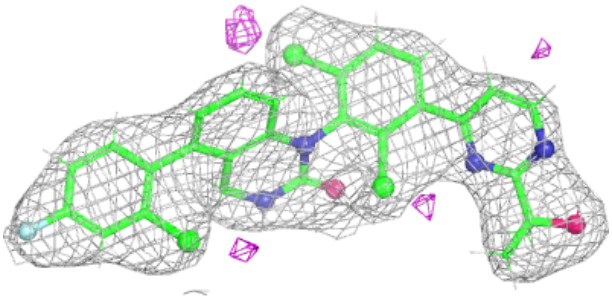


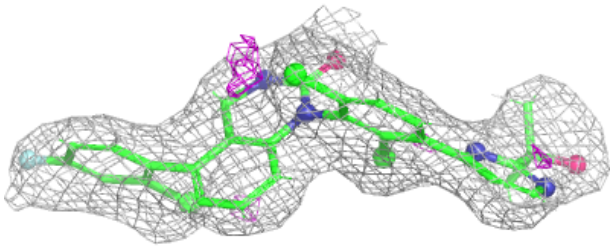


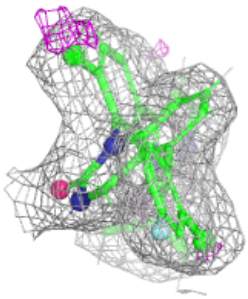


Electron density around A1C0A A 401:

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

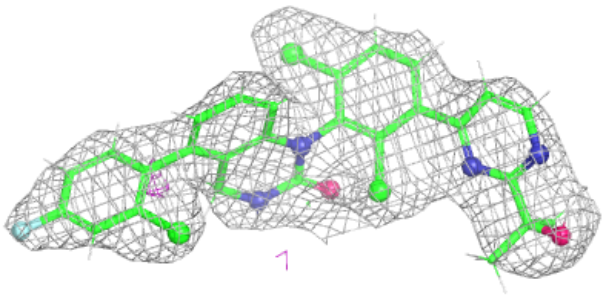


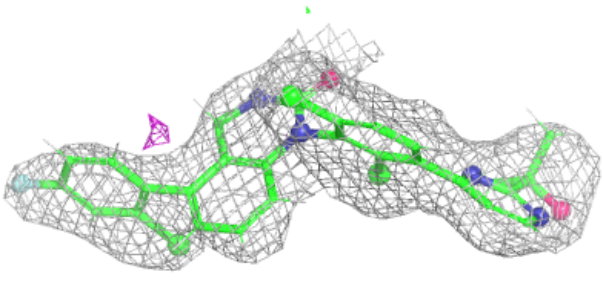


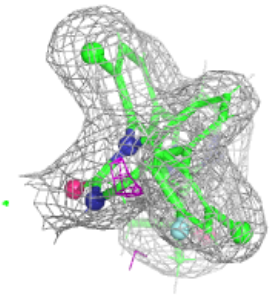


Electron density around A1C0A B 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.