



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:59 pm BST

PDB ID : 4QTD
Title : Structure of human JNK1 in complex with SCH772984 and the AMPPNP-hydrolysed triphosphate revealing the second type-I binding mode
Authors : Chaikuad, A.; Keates, T.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2014-07-07
Resolution : 1.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

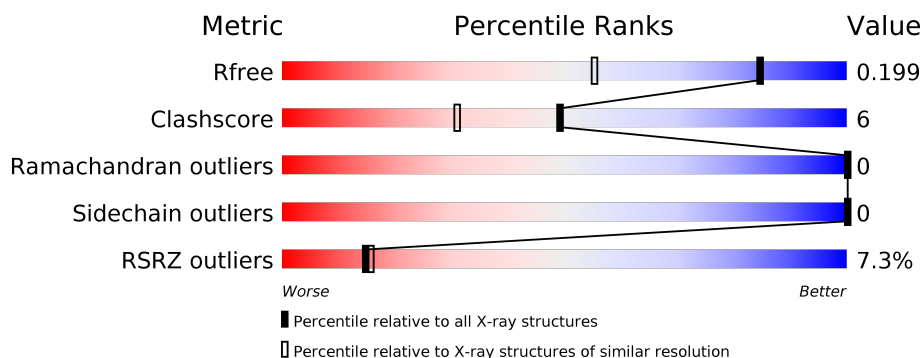
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 on 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	364	

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
2	EDO	A	413	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3521 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mitogen-activated protein kinase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	355	2985	1925	493	541	26	0	23	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P45983

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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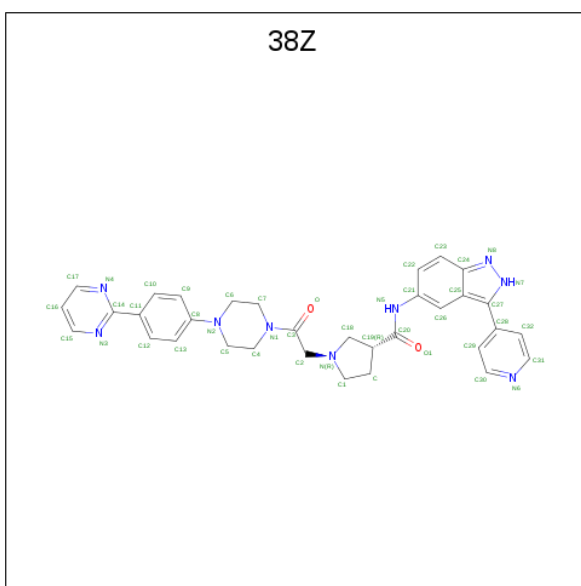
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 8	C 4	O 4	0	1
2	A	1	Total 8	C 4	O 4	0	1
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

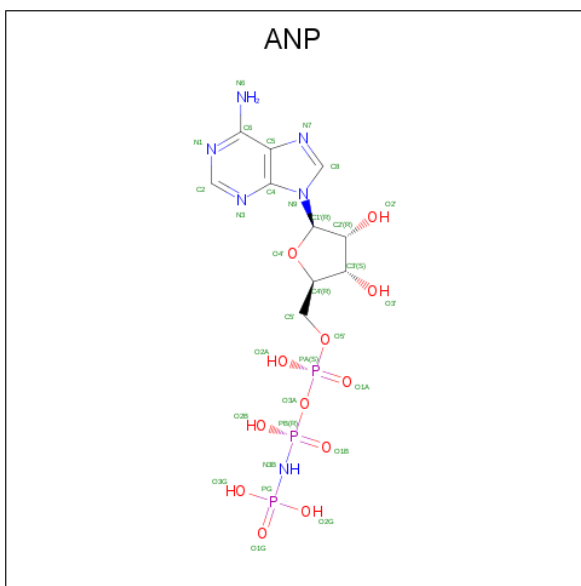
- Molecule 4 is (3R)-1-(2-oxo-2-{4-[4-(pyrimidin-2-yl)phenyl]piperazin-1-yl}ethyl)-N-[3-(pyridin-4-yl)-2H-indazol-5-yl]pyrrolidine-3-carboxamide (three-letter code: 38Z) (formula: $C_{33}H_{33}N_9O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			44	33	9	2		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	N	O	P	0	0
			13	1	9	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0

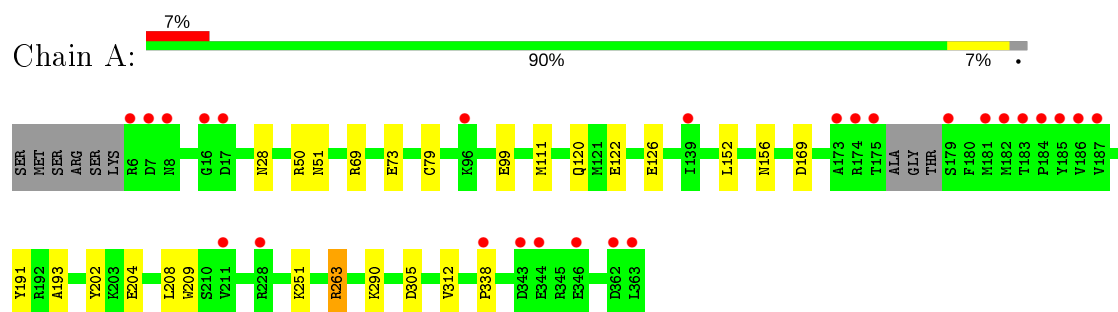
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	367	Total O 367 367	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.95Å 71.55Å 108.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.68 – 1.50 25.75 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (59.68-1.50) 99.9 (25.75-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.166 , 0.192 0.174 , 0.199	Depositor DCC
R_{free} test set	3187 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3521	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EPE, ANP, EDO, 38Z

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	0.80	3/3119 (0.1%)	0.77	3/4216 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	GLU	CD-OE1	7.81	1.34	1.25
1	A	126	GLU	CD-OE2	7.30	1.33	1.25
1	A	191	TYR	CE1-CZ	5.13	1.45	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	A	263	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	A	305	ASP	CB-CG-OD1	5.29	123.06	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2985	0	3045	32	0
2	A	96	0	143	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	18	2	0
4	A	44	0	33	5	0
5	A	13	0	1	0	0
6	A	1	0	0	0	0
7	A	367	0	0	12	0
All	All	3521	0	3240	38	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 6.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:MET:H	4:A:424:38Z:H7	1.28	0.81
1:A:208:LEU:HD21	1:A:312[A]:VAL:HG12	1.70	0.72
1:A:79[B]:CYS:SG	7:A:522:HOH:O	2.43	0.68
1:A:169[A]:ASP:OD2	7:A:778:HOH:O	2.13	0.66
1:A:51:ASN:H	2:A:413:EDO:H22	1.60	0.66
1:A:263:ARG:CD	7:A:716:HOH:O	2.46	0.63
2:A:419:EDO:H12	3:A:423:EPE:H101	1.79	0.63
1:A:263:ARG:HD3	7:A:716:HOH:O	2.02	0.59
1:A:28:ASN:HD22	2:A:412:EDO:H11	1.68	0.57
1:A:204:GLU:HG2	7:A:704:HOH:O	2.05	0.56
1:A:263:ARG:HD2	7:A:716:HOH:O	2.06	0.55
1:A:122:GLU:HB3	2:A:409[B]:EDO:H21	1.88	0.54
1:A:120:GLN:HG3	4:A:424:38Z:C15	2.38	0.53
2:A:419:EDO:H21	7:A:814:HOH:O	2.08	0.53
1:A:28:ASN:ND2	2:A:412:EDO:H11	2.25	0.52
1:A:156[A]:ASN:OD1	4:A:424:38Z:H17	2.11	0.50
1:A:152[A]:LEU:HD12	7:A:779:HOH:O	2.13	0.49
1:A:69:ARG:O	1:A:73:GLU:HG3	2.12	0.49
1:A:51:ASN:H	2:A:413:EDO:C2	2.24	0.48
2:A:419:EDO:H12	3:A:423:EPE:C10	2.42	0.48
1:A:251[B]:LYS:NZ	7:A:561:HOH:O	2.44	0.47
1:A:79[B]:CYS:SG	1:A:338:PRO:HD3	2.55	0.47
2:A:403:EDO:H12	7:A:728:HOH:O	2.15	0.46
1:A:202:TYR:H	2:A:405:EDO:H11	1.81	0.46
1:A:51:ASN:N	2:A:413:EDO:H22	2.28	0.45
1:A:79[B]:CYS:SG	1:A:338:PRO:CD	3.04	0.45
1:A:50[A]:ARG:HB2	2:A:413:EDO:O2	2.18	0.44
1:A:290:LYS:HD3	1:A:290:LYS:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:TYR:H	2:A:405:EDO:C1	2.31	0.43
1:A:208:LEU:HD21	1:A:312[A]:VAL:CG1	2.45	0.42
4:A:424:38Z:H28	4:A:424:38Z:H23	1.84	0.41
4:A:424:38Z:H20	4:A:424:38Z:H19	1.67	0.41
1:A:99[B]:GLU:HG2	7:A:703:HOH:O	2.20	0.41
1:A:263:ARG:HD2	1:A:263:ARG:HA	1.82	0.41
1:A:193:ALA:HA	1:A:209:TRP:CD1	2.55	0.41
1:A:290:LYS:HD2	2:A:415:EDO:H12	2.02	0.41
1:A:204:GLU:CG	7:A:704:HOH:O	2.67	0.40
1:A:50[A]:ARG:HH21	1:A:50[A]:ARG:HG2	1.86	0.40

There are no symmetry-related clashes.

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	374/364 (103%)	368 (98%)	6 (2%)	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	340/328 (104%)	340 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 1 is 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	$\# Z > 2$
2	EDO	A	408[A]	-	3,3,3	0.45	0	2,2,2	0.29	0
2	EDO	A	405	-	3,3,3	0.28	0	2,2,2	1.01	0
2	EDO	A	408[B]	-	3,3,3	0.41	0	2,2,2	0.42	0
2	EDO	A	401	-	3,3,3	0.86	0	2,2,2	0.42	0
2	EDO	A	419	-	3,3,3	0.29	0	2,2,2	0.44	0
2	EDO	A	413	-	3,3,3	0.76	0	2,2,2	0.37	0
3	EPE	A	423	-	15,15,15	1.67	3 (20%)	18,20,20	2.04	4 (22%)
2	EDO	A	403	-	3,3,3	0.58	0	2,2,2	0.64	0
2	EDO	A	421	-	3,3,3	0.53	0	2,2,2	0.29	0
2	EDO	A	415	-	3,3,3	0.48	0	2,2,2	0.28	0
2	EDO	A	418	-	3,3,3	0.39	0	2,2,2	0.50	0
2	EDO	A	402	-	3,3,3	0.22	0	2,2,2	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	420	-	3,3,3	0.35	0	2,2,2	1.12	0
2	EDO	A	417	-	3,3,3	0.38	0	2,2,2	0.51	0
2	EDO	A	414	-	3,3,3	0.46	0	2,2,2	0.20	0
4	38Z	A	424	6	48,50,50	0.74	1 (2%)	62,70,70	2.08	9 (14%)
2	EDO	A	409[A]	-	3,3,3	0.53	0	2,2,2	0.44	0
2	EDO	A	409[B]	-	3,3,3	0.51	0	2,2,2	0.48	0
2	EDO	A	412	-	3,3,3	0.15	0	2,2,2	0.48	0
5	ANP	A	425	6	11,12,33	3.39	5 (45%)	15,20,52	3.60	4 (26%)
2	EDO	A	416	-	3,3,3	0.48	0	2,2,2	0.39	0
2	EDO	A	410	-	3,3,3	0.27	0	2,2,2	0.58	0
2	EDO	A	406	-	3,3,3	0.24	0	2,2,2	0.49	0
2	EDO	A	411	-	3,3,3	0.55	0	2,2,2	0.69	0
2	EDO	A	404	-	3,3,3	0.38	0	2,2,2	0.48	0
2	EDO	A	422	-	3,3,3	0.27	0	2,2,2	0.24	0
2	EDO	A	407	-	3,3,3	0.97	0	2,2,2	1.34	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
2	EDO	A	408[A]	-	-	1/1/1/1	-
2	EDO	A	405	-	-	0/1/1/1	-
2	EDO	A	408[B]	-	-	1/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	A	419	-	-	0/1/1/1	-
2	EDO	A	413	-	-	1/1/1/1	-
3	EPE	A	423	-	-	0/9/19/19	0/1/1/1
2	EDO	A	403	-	-	1/1/1/1	-
2	EDO	A	421	-	-	0/1/1/1	-
2	EDO	A	415	-	-	0/1/1/1	-
2	EDO	A	418	-	-	1/1/1/1	-
2	EDO	A	402	-	-	0/1/1/1	-
2	EDO	A	420	-	-	1/1/1/1	-
2	EDO	A	417	-	-	1/1/1/1	-
2	EDO	A	414	-	-	1/1/1/1	-
4	38Z	A	424	6	-	6/28/47/47	0/7/7/7
2	EDO	A	409[A]	-	-	1/1/1/1	-
2	EDO	A	409[B]	-	-	0/1/1/1	-
2	EDO	A	412	-	-	1/1/1/1	-
5	ANP	A	425	6	-	4/8/12/38	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	416	-	-	1/1/1/1	-
2	EDO	A	410	-	-	0/1/1/1	-
2	EDO	A	406	-	-	0/1/1/1	-
2	EDO	A	411	-	-	1/1/1/1	-
2	EDO	A	404	-	-	1/1/1/1	-
2	EDO	A	422	-	-	1/1/1/1	-
2	EDO	A	407	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	425	ANP	PB-O1B	7.57	1.58	1.46
5	A	425	ANP	PG-O1G	5.09	1.54	1.46
5	A	425	ANP	PB-N3B	4.16	1.74	1.63
3	A	423	EPE	O2S-S	4.08	1.57	1.45
3	A	423	EPE	C10-S	-3.89	1.72	1.77
5	A	425	ANP	PG-N3B	3.52	1.72	1.63
5	A	425	ANP	PB-O3A	2.34	1.62	1.59
3	A	423	EPE	C9-N1	2.08	1.52	1.47
4	A	424	38Z	C26-C25	-2.07	1.38	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	424	38Z	C2-N-C18	10.69	131.35	113.28
5	A	425	ANP	O1G-PG-N3B	-10.43	96.42	111.77
4	A	424	38Z	C19-C18-N	-8.42	93.64	104.40
5	A	425	ANP	O2B-PB-O1B	7.91	126.50	109.92
3	A	423	EPE	O1S-S-C10	-5.71	100.04	106.92
4	A	424	38Z	C2-N-C1	5.37	120.39	113.25
3	A	423	EPE	O2S-S-C10	4.42	112.24	106.92
4	A	424	38Z	C-C19-C18	3.78	107.44	102.45
5	A	425	ANP	O3G-PG-O1G	3.29	121.71	113.45
4	A	424	38Z	C1-N-C18	2.64	106.60	104.02
4	A	424	38Z	C22-C23-C24	-2.49	117.70	120.84
4	A	424	38Z	C19-C20-N5	-2.41	111.48	115.02
5	A	425	ANP	PA-O3A-PB	-2.31	124.48	132.62
4	A	424	38Z	C28-C27-N7	2.29	124.71	120.78
3	A	423	EPE	C7-N4-C3	-2.20	105.61	111.23
3	A	423	EPE	O3S-S-C10	-2.18	102.24	105.77
4	A	424	38Z	C1-C-C19	-2.06	102.48	105.83

There are no chirality outliers.

All (26) torsion outliers are listed below:

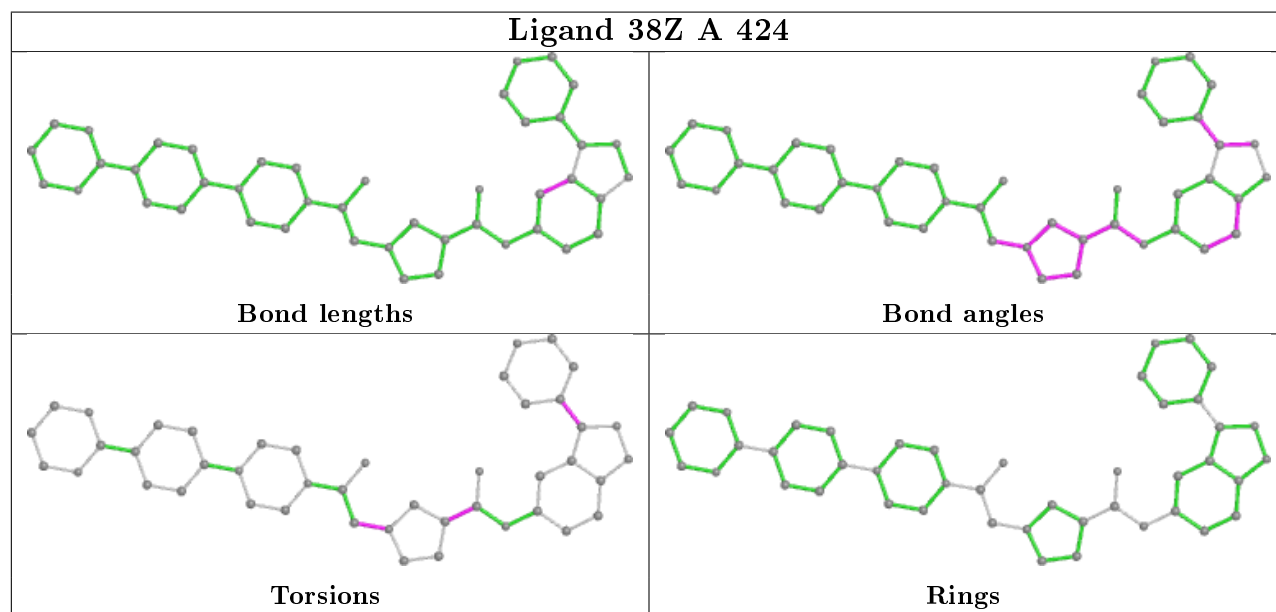
Mol	Chain	Res	Type	Atoms
4	A	424	38Z	C3-C2-N-C18
5	A	425	ANP	PB-N3B-PG-O1G
5	A	425	ANP	PA-O3A-PB-O1B
5	A	425	ANP	PA-O3A-PB-O2B
4	A	424	38Z	C25-C27-C28-C32
2	A	408[B]	EDO	O1-C1-C2-O2
2	A	413	EDO	O1-C1-C2-O2
2	A	418	EDO	O1-C1-C2-O2
2	A	417	EDO	O1-C1-C2-O2
2	A	416	EDO	O1-C1-C2-O2
2	A	411	EDO	O1-C1-C2-O2
2	A	408[A]	EDO	O1-C1-C2-O2
2	A	412	EDO	O1-C1-C2-O2
2	A	401	EDO	O1-C1-C2-O2
2	A	404	EDO	O1-C1-C2-O2
5	A	425	ANP	PG-N3B-PB-O3A
4	A	424	38Z	C25-C27-C28-C29
2	A	403	EDO	O1-C1-C2-O2
2	A	420	EDO	O1-C1-C2-O2
2	A	422	EDO	O1-C1-C2-O2
4	A	424	38Z	C-C19-C20-N5
2	A	407	EDO	O1-C1-C2-O2
2	A	414	EDO	O1-C1-C2-O2
2	A	409[A]	EDO	O1-C1-C2-O2
4	A	424	38Z	C18-C19-C20-O1
4	A	424	38Z	C-C19-C20-O1

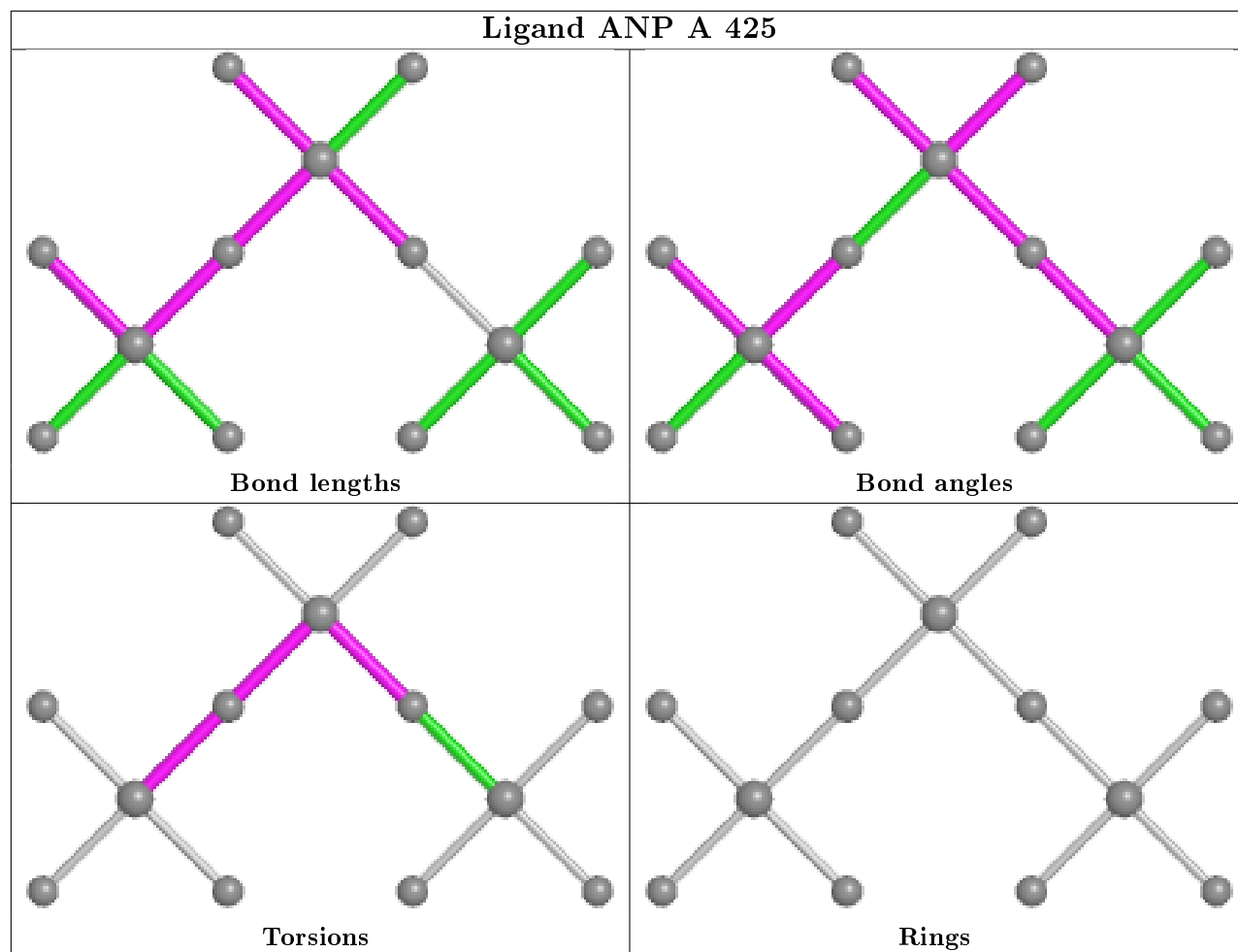
There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	405	EDO	2	0
2	A	419	EDO	3	0
2	A	413	EDO	4	0
3	A	423	EPE	2	0
2	A	403	EDO	1	0
2	A	415	EDO	1	0
4	A	424	38Z	5	0
2	A	409[B]	EDO	1	0
2	A	412	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	355/364 (97%)	0.33	26 (7%) 15 16	9, 19, 44, 67	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	THR	5.4
1	A	185	TYR	5.3
1	A	363	LEU	5.3
1	A	184	PRO	5.0
1	A	17	ASP	4.9
1	A	338	PRO	4.4
1	A	186	VAL	4.4
1	A	343	ASP	3.9
1	A	174	ARG	3.9
1	A	179	SER	3.7
1	A	187	VAL	3.6
1	A	6	ARG	3.4
1	A	7	ASP	3.3
1	A	8	ASN	3.2
1	A	173	ALA	3.0
1	A	139[A]	ILE	2.9
1	A	181	MET	2.9
1	A	183	THR	2.9
1	A	16	GLY	2.7
1	A	182	MET	2.6
1	A	228	ARG	2.6
1	A	96	LYS	2.4
1	A	346	GLU	2.4
1	A	344	GLU	2.3
1	A	362	ASP	2.2
1	A	211	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
2	EDO	A	409[A]	4/4	0.63	0.31	30,31,31,32	4
2	EDO	A	409[B]	4/4	0.63	0.31	28,33,34,34	4
2	EDO	A	421	4/4	0.64	0.18	49,50,50,53	0
2	EDO	A	404	4/4	0.73	0.14	40,43,43,45	0
2	EDO	A	401	4/4	0.74	0.21	32,40,42,42	0
2	EDO	A	407	4/4	0.79	0.19	22,23,29,38	0
2	EDO	A	411	4/4	0.80	0.16	26,32,34,39	0
2	EDO	A	413	4/4	0.80	0.19	23,30,35,36	0
2	EDO	A	410	4/4	0.80	0.14	48,48,51,52	0
2	EDO	A	408[B]	4/4	0.81	0.20	33,33,34,36	4
2	EDO	A	408[A]	4/4	0.81	0.20	45,48,49,51	4
2	EDO	A	405	4/4	0.82	0.22	28,31,37,38	0
2	EDO	A	419	4/4	0.82	0.18	25,29,32,37	0
2	EDO	A	417	4/4	0.83	0.23	44,45,47,54	0
2	EDO	A	416	4/4	0.83	0.16	45,50,50,52	0
2	EDO	A	418	4/4	0.83	0.14	41,41,47,52	0
2	EDO	A	414	4/4	0.86	0.23	49,49,51,54	0
2	EDO	A	402	4/4	0.86	0.21	41,43,44,47	0
2	EDO	A	412	4/4	0.87	0.11	36,37,38,40	0
3	EPE	A	423	15/15	0.87	0.16	19,23,28,34	0
4	38Z	A	424	44/44	0.87	0.15	14,31,55,58	0
2	EDO	A	415	4/4	0.90	0.18	26,30,31,34	0
2	EDO	A	420	4/4	0.91	0.15	32,38,39,41	0
5	ANP	A	425	13/31	0.92	0.18	32,34,39,39	0
2	EDO	A	403	4/4	0.92	0.17	18,26,27,29	0
2	EDO	A	422	4/4	0.93	0.13	29,34,39,42	0
2	EDO	A	406	4/4	0.97	0.09	20,26,31,37	0

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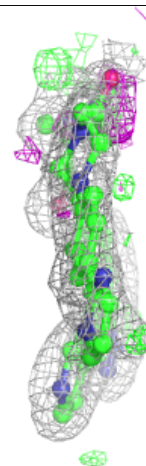
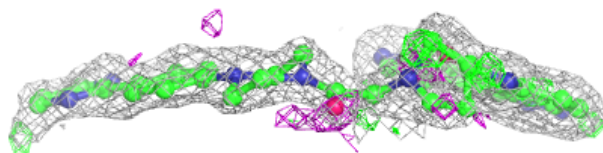
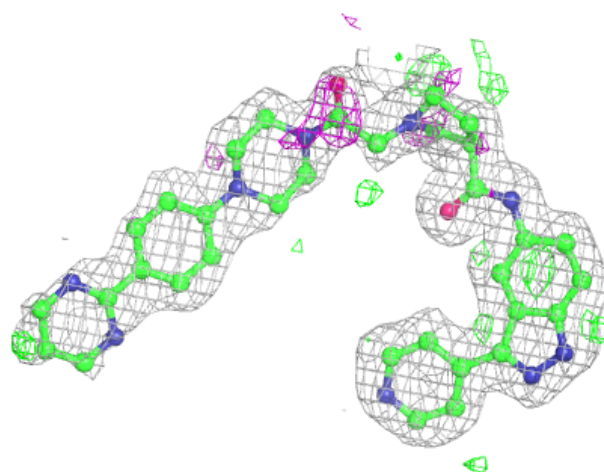
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	A	426	1/1	0.99	0.07	17,17,17,17	0

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.

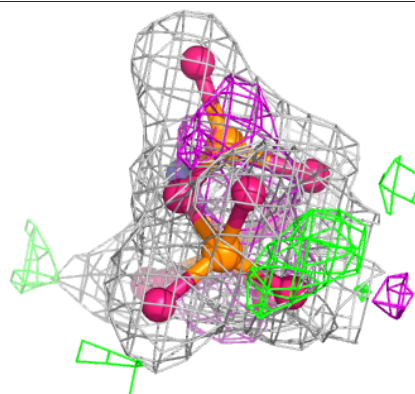
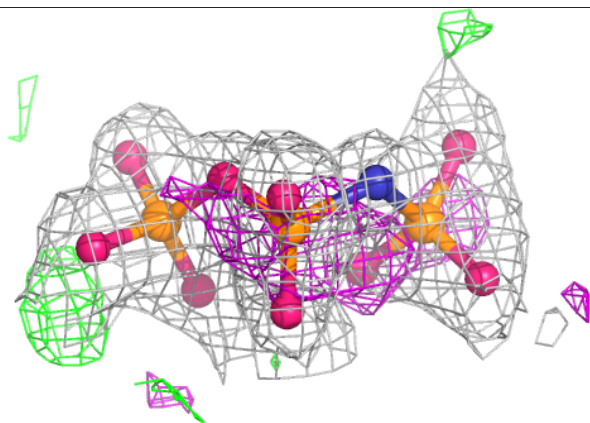
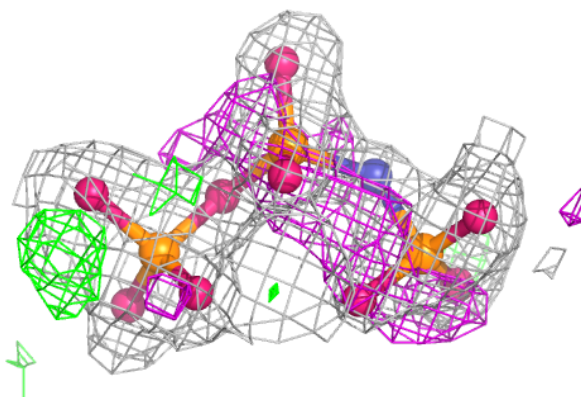
Electron density around 38Z A 424:

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 ANP A 425:

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.