



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:55 pm GMT

PDB ID : 4JQ3
Title : AKR1C2 complex with zomepirac
Authors : Yosaatmadja, Y.; Flanagan, J.U.; Squire, C.J.
Deposited on : 2013-03-19
Resolution : 1.75 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

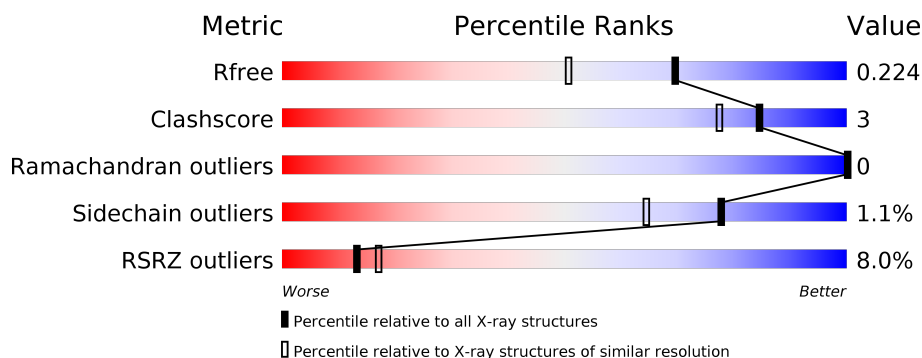
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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. 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	331	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> </div>
1	B	331	<div> <div>10%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	404	-	-	-	X
4	EDO	B	405	-	-	-	X
5	TLA	A	404	-	-	-	X
6	PO4	B	407	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5573 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.

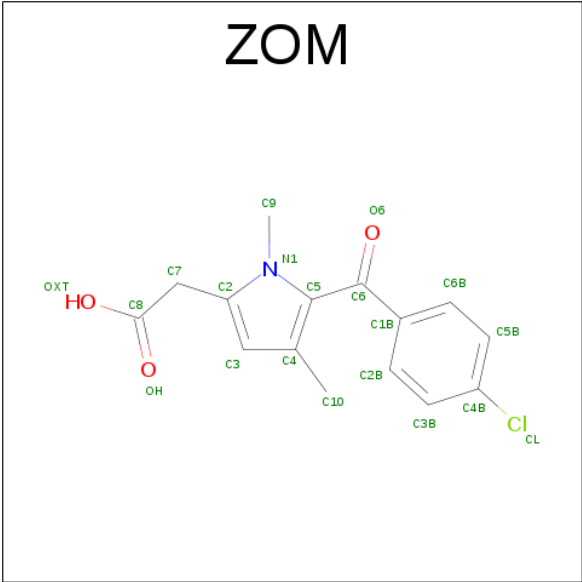
- Molecule 1 is a protein called Aldo-keto reductase family 1 member C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	1	0
			2540	1630	440	459	11			
1	B	318	Total	C	N	O	S	0	2	0
			2553	1638	440	464	11			

There are 16 discrepancies between the modelled and reference sequences:

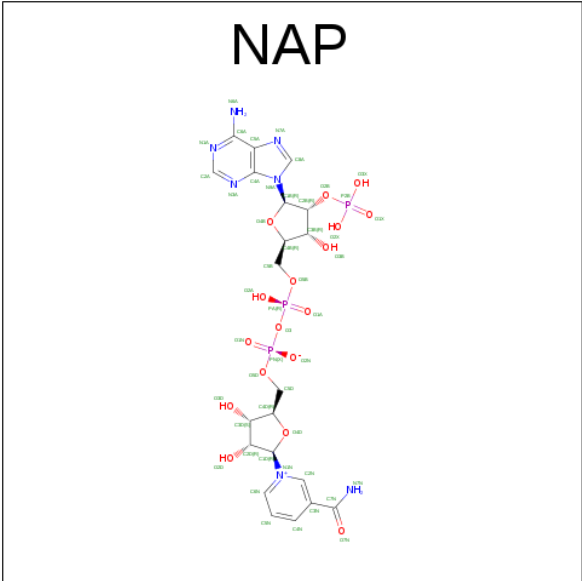
Chain	Residue	Modelled	Actual	Comment	Reference
A	324	LEU	-	EXPRESSION TAG	UNP P52895
A	325	GLU	-	EXPRESSION TAG	UNP P52895
A	326	HIS	-	EXPRESSION TAG	UNP P52895
A	327	HIS	-	EXPRESSION TAG	UNP P52895
A	328	HIS	-	EXPRESSION TAG	UNP P52895
A	329	HIS	-	EXPRESSION TAG	UNP P52895
A	330	HIS	-	EXPRESSION TAG	UNP P52895
A	331	HIS	-	EXPRESSION TAG	UNP P52895
B	324	LEU	-	EXPRESSION TAG	UNP P52895
B	325	GLU	-	EXPRESSION TAG	UNP P52895
B	326	HIS	-	EXPRESSION TAG	UNP P52895
B	327	HIS	-	EXPRESSION TAG	UNP P52895
B	328	HIS	-	EXPRESSION TAG	UNP P52895
B	329	HIS	-	EXPRESSION TAG	UNP P52895
B	330	HIS	-	EXPRESSION TAG	UNP P52895
B	331	HIS	-	EXPRESSION TAG	UNP P52895

- Molecule 2 is [5-(4-CHLOROBENZOYL)-1,4-DIMETHYL-1H-PYRROL-2-YL]ACETIC ACID (three-letter code: ZOM) (formula: C₁₅H₁₄ClNO₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			20	15	1	1	3		
2	B	1	Total	C	Cl	N	O	0	0
			20	15	1	1	3		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

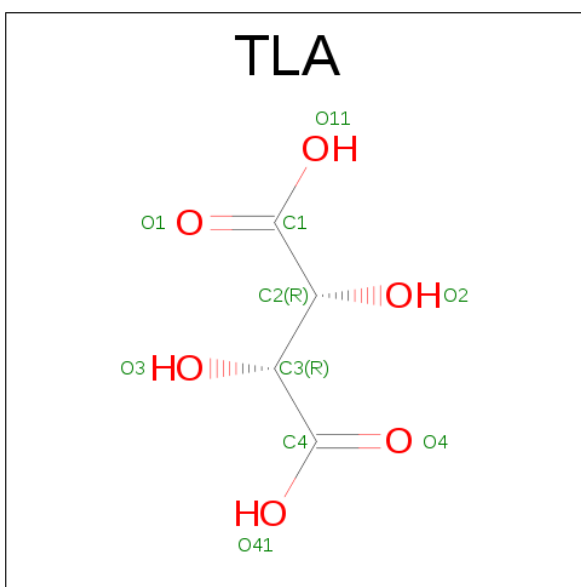
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



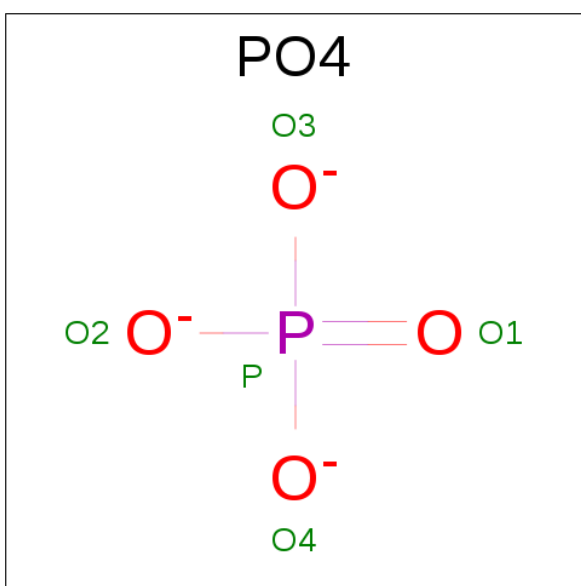
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		

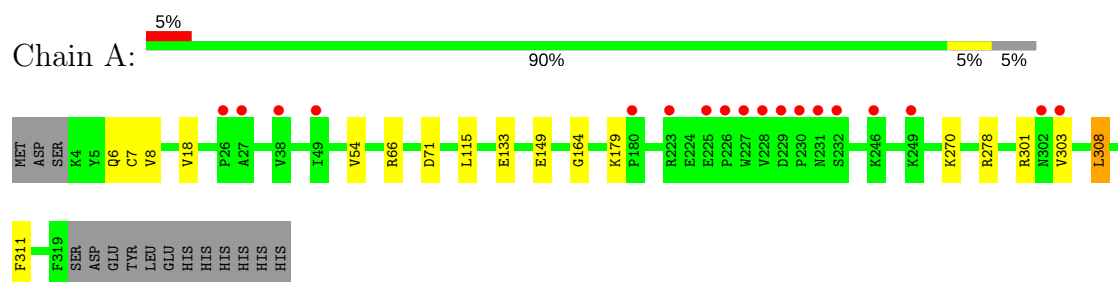
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	145	Total 145	O 145	0	0
7	B	154	Total 154	O 154	0	0

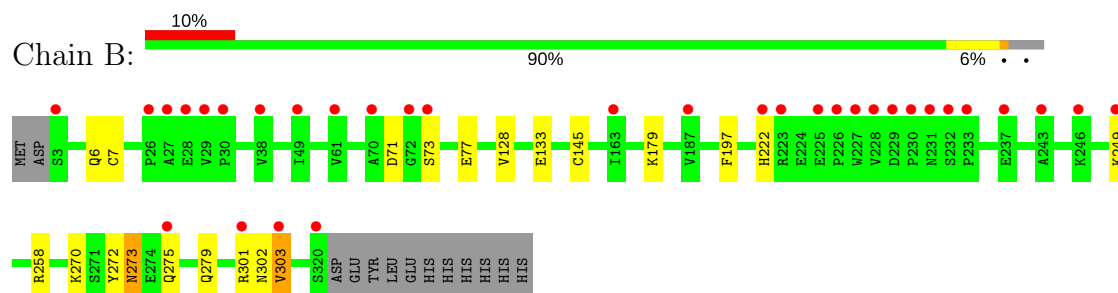
3 Residue-property plots [i](#)

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: Aldo-keto reductase family 1 member C2



- Molecule 1: Aldo-keto reductase family 1 member C2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	143.65Å 143.65Å 203.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.84 – 1.75 19.83 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.84-1.75) 96.6 (19.83-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.162 , 0.224 0.174 , 0.224	Depositor DCC
R_{free} test set	3924 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.6	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	5573	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: PO4, TLA, EDO, NAP, ZOM

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	0.88	1/2600 (0.0%)	0.86	2/3522 (0.1%)
1	B	0.90	1/2613 (0.0%)	0.89	1/3540 (0.0%)
All	All	0.89	2/5213 (0.0%)	0.87	3/7062 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	GLU	CD-OE2	-5.63	1.19	1.25
1	B	279	GLN	CD-OE1	5.10	1.35	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	258	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	71	ASP	CB-CG-OD1	5.16	122.95	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	2540	0	2561	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2553	0	2565	13	0
2	A	20	0	13	1	0
2	B	20	0	13	5	0
3	A	48	0	25	1	0
3	B	48	0	25	1	0
4	A	4	0	6	0	0
4	B	16	0	24	2	0
5	A	10	0	4	0	0
5	B	10	0	4	0	0
6	B	5	0	0	0	0
7	A	145	0	0	3	0
7	B	154	0	0	2	0
All	All	5573	0	5240	28	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 3.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ARG:HG3	1:B:303:VAL:HG13	1.68	0.74
1:A:301:ARG:HG3	1:A:303:VAL:HG23	1.75	0.69
1:B:77:GLU:HB2	7:B:555:HOH:O	1.94	0.67
1:B:301:ARG:HG3	1:B:303:VAL:CG1	2.26	0.66
1:A:308:LEU:HG	1:A:311:PHE:CD2	2.32	0.64
1:A:308:LEU:HG	1:A:311:PHE:HD2	1.62	0.64
2:B:401:ZOM:C1B	2:B:401:ZOM:H10	2.31	0.61
1:A:6[B]:GLN:HG3	1:B:7:CYS:O	1.99	0.61
1:A:7:CYS:O	1:B:6[B]:GLN:HG3	2.01	0.60
2:B:401:ZOM:C2B	2:B:401:ZOM:H10	2.33	0.59
1:B:71:ASP:OD1	1:B:73:SER:HB2	2.03	0.58
7:A:507:HOH:O	4:B:403:EDO:H11	2.11	0.51
1:B:270:LYS:HE2	1:B:272:TYR:CD1	2.46	0.50
1:A:149:GLU:HG3	1:A:179:LYS:HE3	1.94	0.49
2:B:401:ZOM:C8	3:B:402:NAP:C4N	2.93	0.47
1:A:270:LYS:O	3:A:402:NAP:H8A	2.14	0.46
1:B:71:ASP:OD1	1:B:71:ASP:C	2.53	0.46
1:B:273:ASN:OD1	1:B:275:GLN:HB3	2.16	0.46
1:B:145:CYS:HB3	1:B:179:LYS:HD2	1.98	0.45
1:A:66:ARG:HG3	7:A:623:HOH:O	2.16	0.45
2:B:401:ZOM:C10	2:B:401:ZOM:C2B	2.94	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLU:HG2	7:B:638:HOH:O	2.18	0.43
1:B:197:PHE:HD1	1:B:302:ASN:HA	1.84	0.43
7:A:507:HOH:O	4:B:403:EDO:C1	2.68	0.42
1:A:115:LEU:HA	1:A:164:GLY:O	2.19	0.42
2:A:401:ZOM:H9	2:A:401:ZOM:O6	2.18	0.42
1:A:8:VAL:HG13	1:A:18:VAL:CG1	2.51	0.41
1:B:128:VAL:HG21	2:B:401:ZOM:C5B	2.51	0.40

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	315/331 (95%)	306 (97%)	9 (3%)	0	100	100
1	B	318/331 (96%)	311 (98%)	7 (2%)	0	100	100
All	All	633/662 (96%)	617 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	279/293 (95%)	277 (99%)	2 (1%)	87	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	280/293 (96%)	276 (99%)	4 (1%)	71	56
All	All	559/586 (95%)	553 (99%)	6 (1%)	78	64

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	308	LEU
1	B	222	HIS
1	B	249	LYS
1	B	273	ASN
1	B	303	VAL

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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
2	ZOM	A	401	-	17,21,21	2.50	4 (23%)	21,30,30	1.78	7 (33%)
3	NAP	A	402	-	44,52,52	2.14	16 (36%)	51,80,80	2.33	11 (21%)
4	EDO	A	403	-	3,3,3	0.79	0	2,2,2	0.35	0
5	TLA	A	404	-	3,9,9	0.95	0	6,12,12	0.91	0
2	ZOM	B	401	-	17,21,21	2.48	7 (41%)	21,30,30	1.99	8 (38%)
3	NAP	B	402	-	44,52,52	2.42	11 (25%)	51,80,80	2.37	9 (17%)
4	EDO	B	403	-	3,3,3	0.60	0	2,2,2	0.68	0
4	EDO	B	404	-	3,3,3	0.99	0	2,2,2	0.48	0
4	EDO	B	405	-	3,3,3	0.74	0	2,2,2	0.21	0
4	EDO	B	406	-	3,3,3	0.59	0	2,2,2	0.04	0
6	PO4	B	407	-	4,4,4	2.71	2 (50%)	6,6,6	1.83	2 (33%)
5	TLA	B	408	-	3,9,9	1.44	0	6,12,12	2.20	3 (50%)

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	ZOM	A	401	-	-	0/5/12/12	0/2/2/2
3	NAP	A	402	-	-	0/27/67/67	0/5/5/5
4	EDO	A	403	-	-	0/1/1/1	0/0/0/0
5	TLA	A	404	-	-	0/4/12/12	0/0/0/0
2	ZOM	B	401	-	-	0/5/12/12	0/2/2/2
3	NAP	B	402	-	-	0/27/67/67	0/5/5/5
4	EDO	B	403	-	-	0/1/1/1	0/0/0/0
4	EDO	B	404	-	-	0/1/1/1	0/0/0/0
4	EDO	B	405	-	-	0/1/1/1	0/0/0/0
4	EDO	B	406	-	-	0/1/1/1	0/0/0/0
6	PO4	B	407	-	-	0/0/0/0	0/0/0/0
5	TLA	B	408	-	-	0/4/12/12	0/0/0/0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ZOM	C5-C6	-5.87	1.40	1.50
2	B	401	ZOM	C5-C6	-5.61	1.41	1.50
2	A	401	ZOM	C1B-C6	-5.39	1.40	1.49
2	B	401	ZOM	C1B-C6	-4.85	1.41	1.49
3	A	402	NAP	C3N-C7N	-4.83	1.43	1.50
3	B	402	NAP	C3N-C7N	-4.40	1.43	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ZOM	C3-C2	-4.39	1.32	1.39
2	B	401	ZOM	C3-C2	-3.00	1.34	1.39
3	B	402	NAP	C5A-C4A	-2.54	1.34	1.40
3	A	402	NAP	PN-O1N	-2.27	1.42	1.50
3	A	402	NAP	C5A-C4A	-2.27	1.35	1.40
6	B	407	PO4	P-O2	-2.19	1.46	1.54
3	A	402	NAP	P2B-O2X	-2.12	1.46	1.54
2	B	401	ZOM	C5-C4	-2.11	1.35	1.40
3	A	402	NAP	O3B-C3B	-2.11	1.38	1.43
3	A	402	NAP	C3D-C4D	2.01	1.58	1.53
3	B	402	NAP	C5B-C4B	2.09	1.58	1.51
3	A	402	NAP	O3D-C3D	2.15	1.47	1.43
3	A	402	NAP	C2D-C3D	2.23	1.59	1.53
2	B	401	ZOM	C6B-C1B	2.33	1.43	1.39
3	B	402	NAP	PN-O5D	2.39	1.69	1.59
2	B	401	ZOM	C9-N1	2.54	1.53	1.48
3	A	402	NAP	C2D-C1D	2.57	1.57	1.53
3	A	402	NAP	PA-O5B	2.71	1.70	1.59
3	A	402	NAP	C2A-N1A	2.71	1.39	1.33
3	A	402	NAP	C5B-C4B	2.76	1.60	1.51
2	A	401	ZOM	C4B-CL	2.86	1.80	1.74
3	B	402	NAP	P2B-O2B	2.91	1.64	1.59
3	A	402	NAP	O4B-C1B	2.98	1.45	1.41
2	B	401	ZOM	C4B-CL	3.52	1.82	1.74
3	B	402	NAP	C3D-C4D	3.55	1.62	1.53
3	B	402	NAP	C6N-N1N	3.62	1.44	1.35
3	A	402	NAP	C6N-N1N	3.91	1.45	1.35
3	B	402	NAP	PA-O5B	3.93	1.75	1.59
3	B	402	NAP	C2A-N1A	4.02	1.41	1.33
6	B	407	PO4	P-O1	4.81	1.60	1.50
3	A	402	NAP	C2A-N3A	5.33	1.41	1.32
3	B	402	NAP	C2A-N3A	5.40	1.41	1.32
3	A	402	NAP	O4D-C1D	6.49	1.50	1.41
3	B	402	NAP	O4D-C1D	9.68	1.54	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAP	N3A-C2A-N1A	-12.40	118.06	128.86
3	A	402	NAP	N3A-C2A-N1A	-12.11	118.31	128.86
3	B	402	NAP	O2A-PA-O5B	-5.26	83.29	108.14
3	A	402	NAP	O2A-PA-O5B	-4.62	86.33	108.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAP	C4D-O4D-C1D	-4.54	104.94	109.77
3	B	402	NAP	O5B-PA-O1A	-4.24	92.14	109.25
2	B	401	ZOM	O6-C6-C1B	-3.95	113.88	120.14
3	A	402	NAP	O5B-PA-O1A	-3.87	93.62	109.25
3	A	402	NAP	C4D-O4D-C1D	-3.65	105.88	109.77
2	A	401	ZOM	O6-C6-C1B	-3.63	114.40	120.14
6	B	407	PO4	O4-P-O1	-3.34	96.74	110.97
2	B	401	ZOM	C10-C4-C5	-3.03	124.03	128.50
5	B	408	TLA	C1-C2-C3	-2.79	107.09	113.11
2	A	401	ZOM	C10-C4-C3	-2.71	119.96	124.93
3	A	402	NAP	O3B-C3B-C4B	-2.42	104.02	111.09
2	A	401	ZOM	C5B-C6B-C1B	-2.19	118.34	120.79
2	A	401	ZOM	C7-C2-C3	-2.14	124.65	130.40
2	B	401	ZOM	C8-C7-C2	-2.08	109.99	113.81
3	B	402	NAP	C5A-C6A-N6A	-2.07	116.25	120.47
2	B	401	ZOM	C3B-C2B-C1B	-2.05	118.50	120.79
3	B	402	NAP	C3N-C2N-N1N	2.01	122.45	120.43
2	B	401	ZOM	O6-C6-C5	2.06	122.57	120.12
2	B	401	ZOM	C2B-C3B-C4B	2.08	121.46	119.24
2	A	401	ZOM	C6B-C5B-C4B	2.09	121.46	119.24
3	B	402	NAP	O4D-C4D-C5D	2.12	116.56	109.40
5	B	408	TLA	O3-C3-C2	2.23	115.59	108.88
3	B	402	NAP	O2A-PA-O1A	2.25	123.93	112.28
3	A	402	NAP	O5D-PN-O1N	2.25	118.34	109.25
3	A	402	NAP	O2A-PA-O1A	2.30	124.20	112.28
6	B	407	PO4	O4-P-O2	2.31	116.40	107.90
2	A	401	ZOM	C9-N1-C2	2.45	126.50	124.09
3	A	402	NAP	O2N-PN-O1N	2.47	125.06	112.28
3	A	402	NAP	C5N-C4N-C3N	2.60	123.41	120.35
3	B	402	NAP	O2N-PN-O1N	2.76	126.58	112.28
3	A	402	NAP	O4B-C4B-C5B	2.88	119.14	109.40
3	A	402	NAP	C2B-C3B-C4B	2.89	108.51	101.95
2	B	401	ZOM	C1B-C6-C5	3.13	123.04	119.46
2	A	401	ZOM	C1B-C6-C5	3.21	123.13	119.46
5	B	408	TLA	O2-C2-C3	3.69	119.99	108.88
2	B	401	ZOM	C9-N1-C2	3.96	127.97	124.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ZOM	1	0
3	A	402	NAP	1	0
2	B	401	ZOM	5	0
3	B	402	NAP	1	0
4	B	403	EDO	2	0

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	316/331 (95%)	0.27	18 (5%) 24 31	22, 32, 54, 80	13 (4%)
1	B	318/331 (96%)	0.35	33 (10%) 7 10	17, 30, 64, 91	7 (2%)
All	All	634/662 (95%)	0.31	51 (8%) 13 17	17, 31, 60, 91	20 (3%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	PRO	5.9
1	B	226	PRO	4.8
1	A	231	ASN	4.7
1	B	320	SER	4.6
1	A	302	ASN	4.6
1	B	231	ASN	4.5
1	A	230	PRO	4.4
1	A	229	ASP	4.1
1	B	232	SER	4.1
1	B	230	PRO	4.0
1	A	225	GLU	3.9
1	A	232	SER	3.8
1	A	227	TRP	3.8
1	B	30	PRO	3.7
1	A	27	ALA	3.7
1	B	29	VAL	3.6
1	B	38	VAL	3.4
1	B	275	GLN	3.4
1	B	28	GLU	3.4
1	B	225	GLU	3.3
1	B	3	SER	3.1
1	B	246	LYS	3.0
1	B	229	ASP	2.9
1	B	49	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	227	TRP	2.8
1	B	61	VAL	2.8
1	B	163	ILE	2.7
1	B	73	SER	2.7
1	B	237	GLU	2.7
1	B	70	ALA	2.7
1	B	303	VAL	2.5
1	A	246	LYS	2.5
1	A	180	PRO	2.5
1	B	72	GLY	2.5
1	A	49	ILE	2.5
1	B	26	PRO	2.4
1	B	249	LYS	2.4
1	A	303	VAL	2.4
1	B	27	ALA	2.3
1	A	249	LYS	2.3
1	B	243	ALA	2.2
1	B	222	HIS	2.2
1	A	26	PRO	2.2
1	B	228	VAL	2.2
1	B	301	ARG	2.2
1	B	233	PRO	2.2
1	B	223	ARG	2.2
1	A	228	VAL	2.1
1	A	38	VAL	2.1
1	B	187	VAL	2.1
1	A	223	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	B	404	4/4	0.84	0.11	2.39	36,36,38,43	0
5	TLA	A	404	10/10	0.82	0.14	2.16	37,45,62,64	0
4	EDO	B	405	4/4	0.84	0.18	2.14	48,51,51,53	0
3	NAP	B	402	48/48	0.91	0.15	1.33	27,56,71,76	0
3	NAP	A	402	48/48	0.94	0.13	1.25	26,38,46,53	0
2	ZOM	B	401	20/20	0.85	0.15	0.92	34,44,56,57	0
2	ZOM	A	401	20/20	0.87	0.14	0.82	37,45,58,61	0
4	EDO	A	403	4/4	0.97	0.10	0.16	24,25,34,34	0
4	EDO	B	406	4/4	0.96	0.08	-0.22	28,29,36,37	0
6	PO4	B	407	5/5	0.92	0.24	-	41,51,56,57	5
5	TLA	B	408	10/10	0.75	0.29	-	34,51,59,69	0
4	EDO	B	403	4/4	0.81	0.19	-	44,54,59,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.