



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 08:53 pm GMT

PDB ID : 4JQA
Title : AKR1C2 complex with mefenamic acid
Authors : Yosaatmadja, Y.; Flanagan, J.U.; Squire, C.J.
Deposited on : 2013-03-20
Resolution : 1.45 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

<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

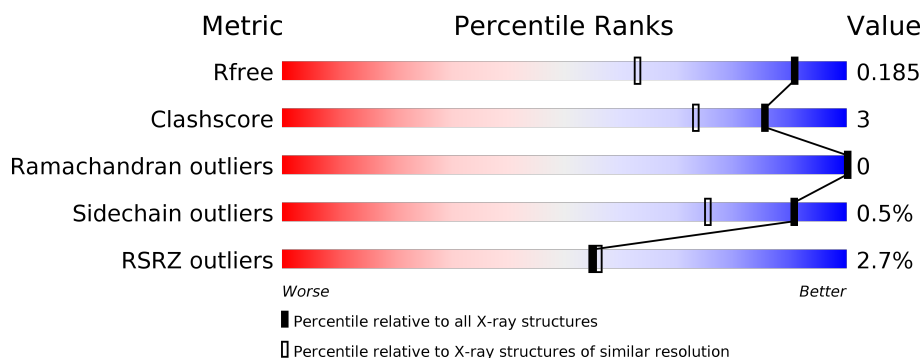
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1510 (1.48-1.44)
Clashscore	112137	1573 (1.48-1.44)
Ramachandran outliers	110173	1555 (1.48-1.44)
Sidechain outliers	110143	1555 (1.48-1.44)
RSRZ outliers	101464	1516 (1.48-1.44)

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>3%</div> <div> <div></div> <div>90%</div> <div>5% • 5%</div> </div> </div>
1	B	331	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>5% •</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
2	ID8	A	401	-	-	-	X
2	ID8	B	401	-	-	-	X
4	EDO	B	405	-	-	-	X
6	TLA	B	403	-	-	-	X
7	PO4	B	407	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5826 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.

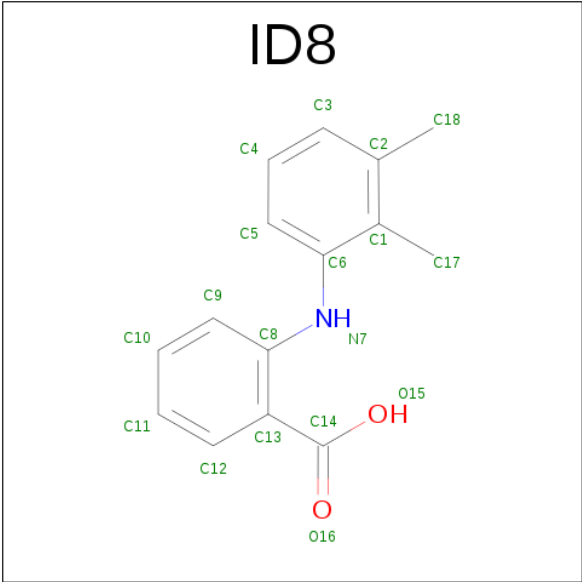
- Molecule 1 is a protein called Aldo-keto reductase family 1 member C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	2	8	0
			2588	1662	443	472	11			
1	B	317	Total	C	N	O	S	3	6	0
			2573	1651	446	465	11			

There are 16 discrepancies between the modelled and reference sequences:

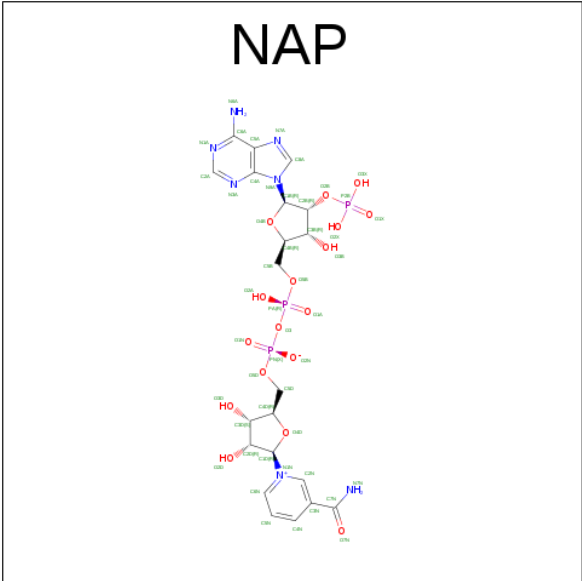
Chain	Residue	Modelled	Actual	Comment	Reference
A	324	LEU	-	EXPRESSION TAG	UNP P52895
A	325	GLU	-	EXPRESSION TAG	UNP P52895
A	326	HIS	-	EXPRESSION TAG	UNP P52895
A	327	HIS	-	EXPRESSION TAG	UNP P52895
A	328	HIS	-	EXPRESSION TAG	UNP P52895
A	329	HIS	-	EXPRESSION TAG	UNP P52895
A	330	HIS	-	EXPRESSION TAG	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 2-[(2,3-DIMETHYLPHENYL)AMINO]BENZOIC ACID (three-letter code: ID8) (formula: C₁₅H₁₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	15	1	2		
2	B	1	Total	C	N	O	0	0
			18	15	1	2		

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



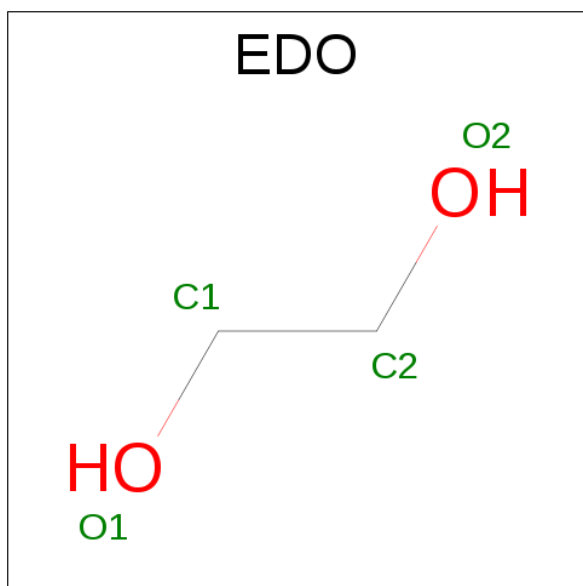
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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: $C_2H_6O_2$).

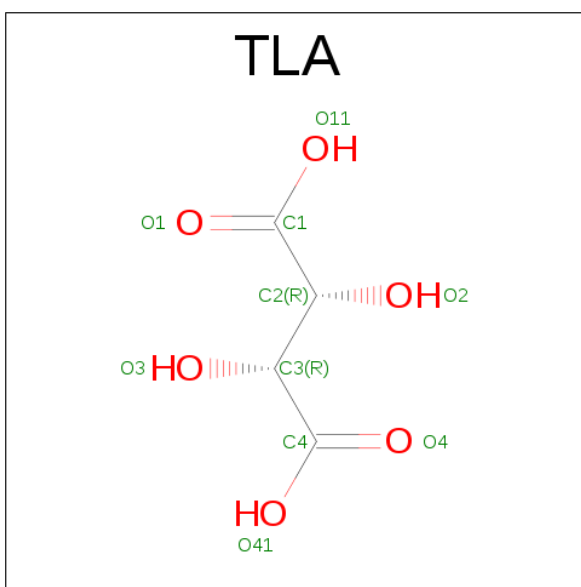


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

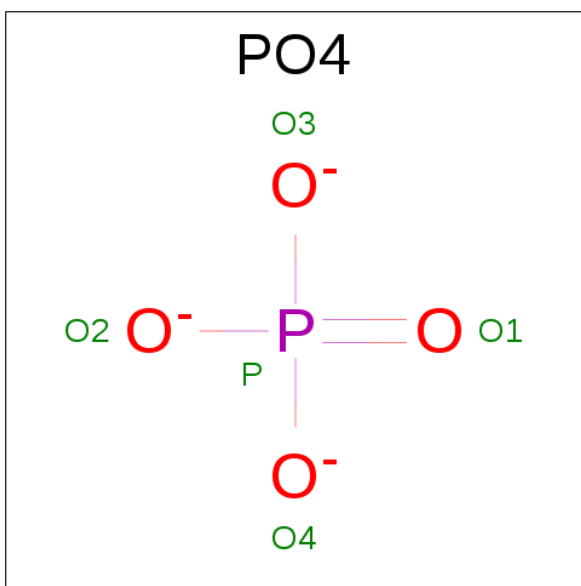
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	255	Total 255	O 255	0	0
8	B	246	Total 246	O 246	0	0

- 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	144.98Å 144.98Å 201.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 1.45 19.90 – 1.45	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.90-1.45) 96.5 (19.90-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.144 , 0.184 0.153 , 0.185	Depositor DCC
R_{free} test set	6934 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5826	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: ID8, NA, PO4, EDO, TLA, NAP

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	1.03	1/2657 (0.0%)	1.07	13/3599 (0.4%)
1	B	1.05	4/2641 (0.2%)	1.08	12/3577 (0.3%)
All	All	1.04	5/5298 (0.1%)	1.07	25/7176 (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
1	B	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	GLU	CG-CD	5.78	1.60	1.51
1	B	171	ARG	CZ-NH1	5.44	1.40	1.33
1	B	110	TYR	CE1-CZ	-5.20	1.31	1.38
1	B	46	PHE	CG-CD1	5.13	1.46	1.38
1	A	101	ARG	CZ-NH1	5.04	1.39	1.33

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ARG	NE-CZ-NH1	10.93	125.76	120.30
1	B	171	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	A	101	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	A	200	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	200	ARG	NE-CZ-NH1	9.63	125.11	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	301[A]	ARG	Mainchain
1	B	301[B]	ARG	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2588	0	2604	12	0
1	B	2573	0	2595	10	0
2	A	18	0	14	1	0
2	B	18	0	14	1	0
3	A	48	0	24	3	0
3	B	48	0	25	9	0
4	A	4	0	6	0	0
4	B	12	0	18	0	0
5	A	1	0	0	0	0
6	B	10	0	5	0	0
7	B	5	0	0	0	0
8	A	255	0	0	4	0
8	B	246	0	0	2	0
All	All	5826	0	5305	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.

The worst 5 of 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)
3:B:402:NAP:O2B	3:B:402:NAP:C2B	1.71	1.37
3:B:402:NAP:P2B	3:B:402:NAP:C2B	2.74	0.76
1:A:301:ARG:HG3	1:A:303:VAL:HG23	1.74	0.70
1:A:222:HIS:CE1	1:A:270:LYS:HD2	2.31	0.65
1:A:200:ARG:HD3	1:A:200:ARG:O	1.99	0.63

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	322/331 (97%)	315 (98%)	7 (2%)	0	100	100
1	B	321/331 (97%)	316 (98%)	5 (2%)	0	100	100
All	All	643/662 (97%)	631 (98%)	12 (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	285/293 (97%)	284 (100%)	1 (0%)	93	82
1	B	282/293 (96%)	279 (99%)	3 (1%)	78	48
All	All	567/586 (97%)	563 (99%)	4 (1%)	91	66

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	B	36	GLU
1	B	301[A]	ARG
1	B	301[B]	ARG

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	ID8	A	401	-	16,19,19	2.53	5 (31%)	22,26,26	1.64	4 (18%)
3	NAP	A	402	5	44,52,52	1.44	3 (6%)	51,80,80	2.02	13 (25%)
4	EDO	A	403	-	3,3,3	0.70	0	2,2,2	0.11	0
2	ID8	B	401	-	16,19,19	1.80	3 (18%)	22,26,26	1.60	5 (22%)
3	NAP	B	402	-	44,52,52	2.33	15 (34%)	51,80,80	2.33	16 (31%)
6	TLA	B	403	-	3,9,9	0.68	0	6,12,12	2.12	1 (16%)
4	EDO	B	404	-	3,3,3	0.67	0	2,2,2	0.19	0
4	EDO	B	405	-	3,3,3	0.92	0	2,2,2	0.99	0
4	EDO	B	406	-	3,3,3	0.94	0	2,2,2	0.38	0
7	PO4	B	407	-	4,4,4	2.50	2 (50%)	6,6,6	1.57	2 (33%)

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	ID8	A	401	-	-	0/4/8/8	0/2/2/2
3	NAP	A	402	5	-	0/27/67/67	0/5/5/5
4	EDO	A	403	-	-	0/1/1/1	0/0/0/0
2	ID8	B	401	-	-	0/4/8/8	0/2/2/2
3	NAP	B	402	-	-	0/27/67/67	0/5/5/5
6	TLA	B	403	-	-	0/4/12/12	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
7	PO4	B	407	-	-	0/0/0/0	0/0/0/0

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ID8	C17-C1	-7.27	1.36	1.51
2	B	401	ID8	C17-C1	-5.16	1.41	1.51
3	A	402	NAP	C3N-C7N	-4.64	1.43	1.50
2	A	401	ID8	C18-C2	-3.79	1.43	1.51
2	B	401	ID8	C18-C2	-3.41	1.44	1.51

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAP	N3A-C2A-N1A	-7.98	121.91	128.86
3	A	402	NAP	C4B-O4B-C1B	-6.47	102.88	109.77
3	B	402	NAP	O2B-P2B-O1X	-5.66	87.09	109.26
3	A	402	NAP	C4A-C5A-N7A	-4.93	104.64	109.41
6	B	403	TLA	O2-C2-C1	-4.73	99.62	111.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ID8	1	0
3	A	402	NAP	3	0
2	B	401	ID8	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	NAP	9	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.13	9 (2%) 53 54	13, 19, 33, 46	9 (2%)
1	B	317/331 (95%)	0.19	8 (2%) 58 59	10, 17, 34, 51	8 (2%)
All	All	633/662 (95%)	0.16	17 (2%) 55 56	10, 18, 33, 51	17 (2%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	ASN	3.8
1	B	3	SER	3.4
1	A	303	VAL	3.3
1	B	301[A]	ARG	3.0
1	B	49[A]	ILE	2.9

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(\AA^2)	Q<0.9
2	ID8	B	401	18/18	0.93	0.13	7.10	15,25,33,43	0
2	ID8	A	401	18/18	0.91	0.14	4.99	16,24,33,39	0
6	TLA	B	403	10/10	0.86	0.14	4.54	23,27,36,47	0
4	EDO	B	405	4/4	0.93	0.12	3.15	21,25,25,28	0
4	EDO	B	406	4/4	0.88	0.14	0.74	27,29,30,32	0
4	EDO	B	404	4/4	0.96	0.10	0.60	15,15,18,21	0
3	NAP	B	402	48/48	0.96	0.09	-0.18	12,20,34,41	0
4	EDO	A	403	4/4	0.97	0.08	-0.54	14,16,19,20	0
3	NAP	A	402	48/48	0.97	0.07	-0.83	12,19,26,28	0
5	NA	A	404	1/1	0.91	0.15	-	42,42,42,42	0
7	PO4	B	407	5/5	0.83	0.22	-	31,39,60,65	5

6.5 Other polymers [i](#)

There are no such residues in this entry.