wwPDB X-ray Structure Validation Summary Report (i)

Feb 13, 2017 – 08:48 pm GMT

PDB ID	:	4JQ2
Title	:	AKR1C2 complex with sulindac
Authors	:	Yosaatmadja, Y.; Flanagan, J.U.; Squire, C.J.
Deposited on	:	2013-03-19
Resolution	:	1.75 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

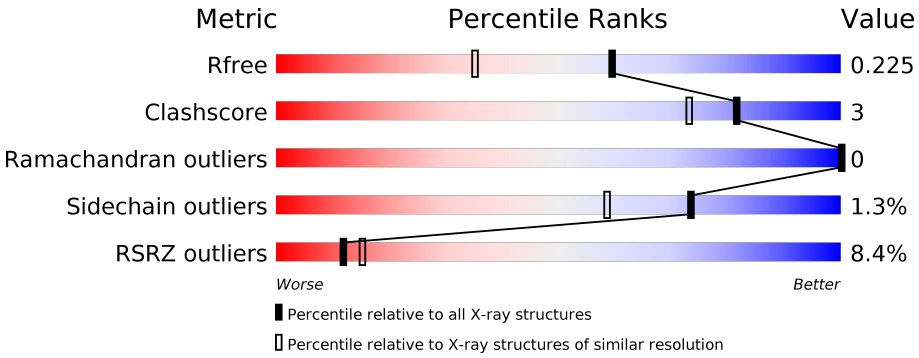
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance (i)

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 <=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	4% 89% 6% 5%
1	B	331	12% 90% 6% .

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	SUZ	A	401	-	-	-	X
4	EDO	B	503	-	-	-	X
4	EDO	B	504	-	-	X	-
5	TLA	A	405	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5630 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.

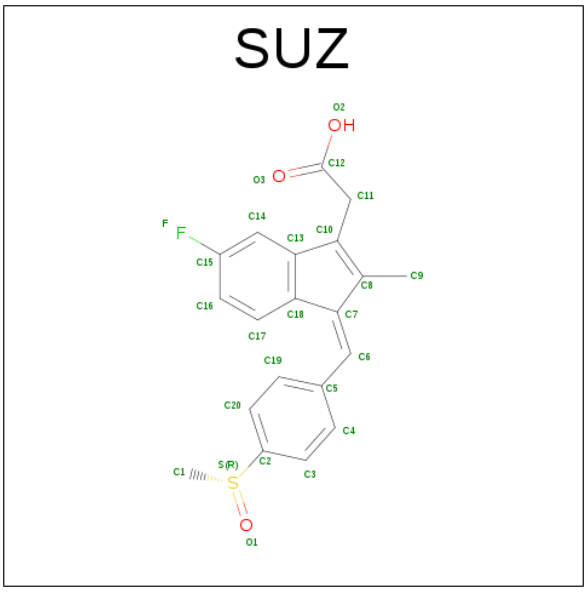
- Molecule 1 is a protein called Aldo-keto reductase family 1 member C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	5	0
			2570	1649	448	462	11			
1	B	318	Total	C	N	O	S	0	5	0
			2572	1646	449	465	12			

There are 16 discrepancies between the modelled and reference sequences:

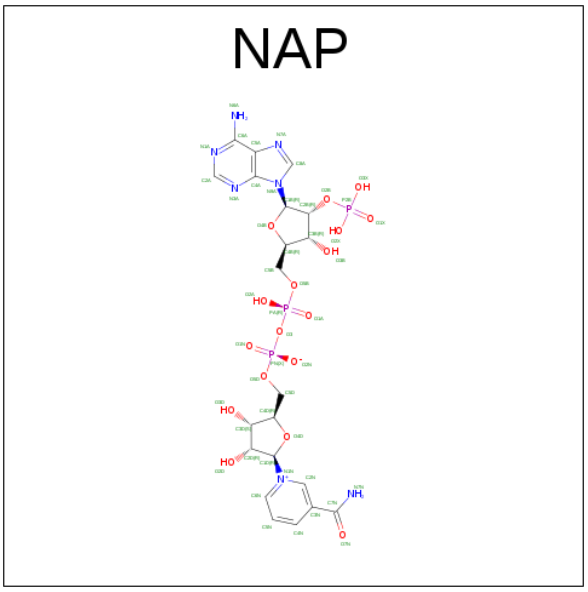
Chain	Residue	Modelled	Actual	Comment	Reference
A	324	LEU	-	EXPRESSION TAG	UNP P52895
A	325	GLU	-	EXPRESSION TAG	UNP P52895
A	326	HIS	-	EXPRESSION TAG	UNP P52895
A	327	HIS	-	EXPRESSION TAG	UNP P52895
A	328	HIS	-	EXPRESSION TAG	UNP P52895
A	329	HIS	-	EXPRESSION TAG	UNP P52895
A	330	HIS	-	EXPRESSION TAG	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 [(1Z)-5-FLUORO-2-METHYL-1-{4-[METHYLSULFINYL]BENZYLIDENE}-1H-INDEN-3-YL]ACETIC ACID (three-letter code: SUZ) (formula: $C_{20}H_{17}FO_3S$).



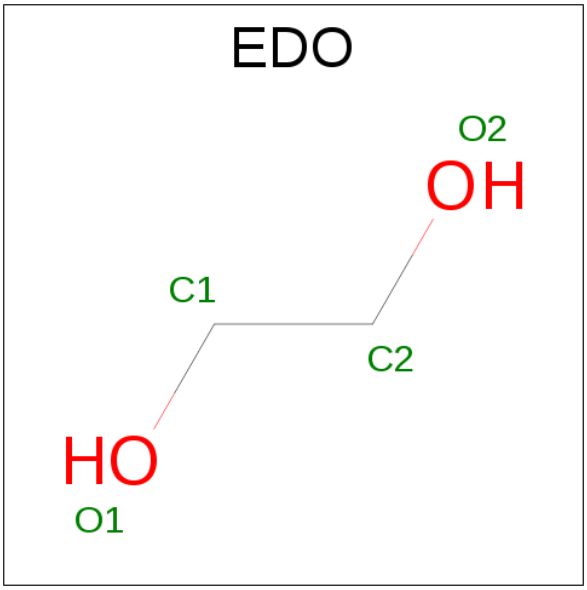
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	O	S	0	0
			25	20	1	3	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



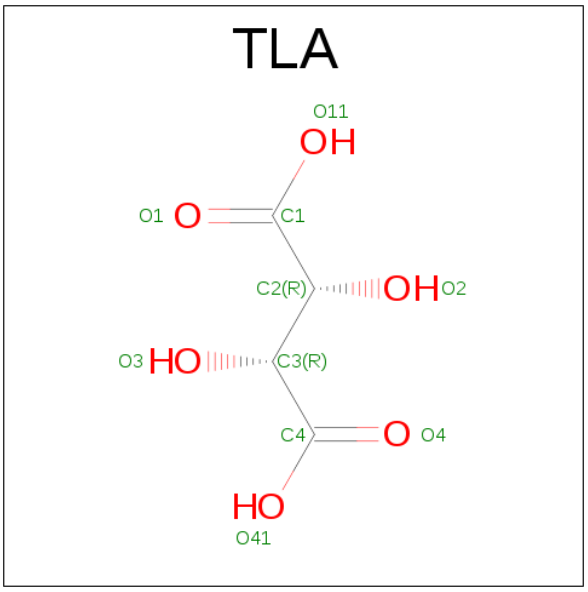
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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



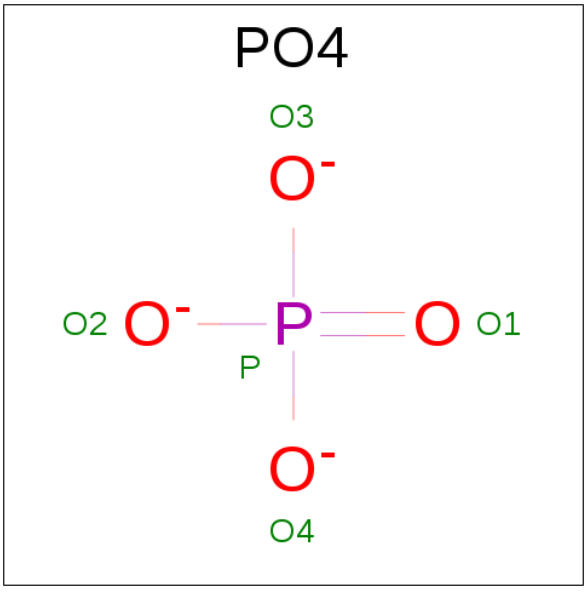
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- 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 10 4 6	0	0

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



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

- Molecule 7 is water.

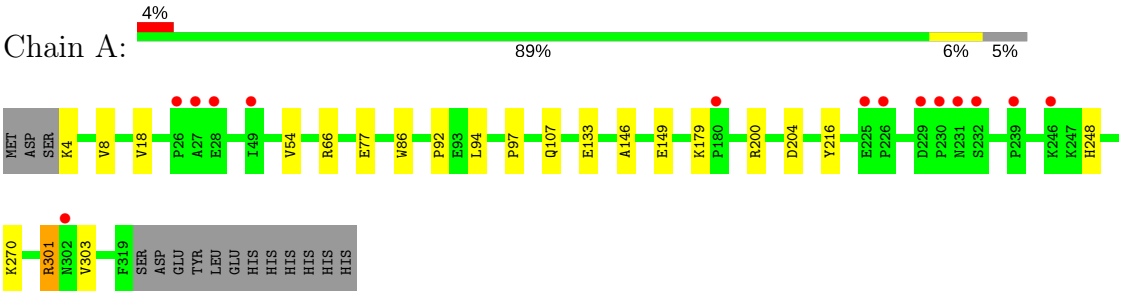
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	164	Total O 164 164	0	0
7	B	168	Total O 168 168	0	0

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.

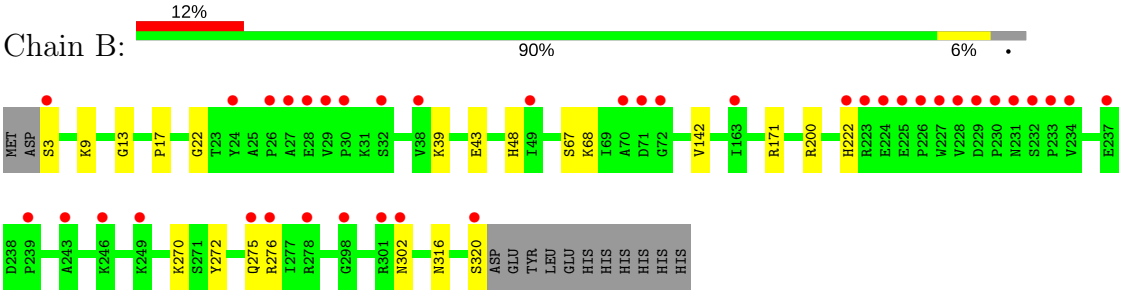
• Molecule 1: Aldo-keto reductase family 1 member C2

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	143.16Å 143.16Å 204.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.79 – 1.75 19.78 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.79-1.75) 99.0 (19.78-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.163 , 0.223 0.172 , 0.225	Depositor DCC
R_{free} test set	4023 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5630	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: PO4, TLA, EDO, NAP, SUZ

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	0.85	1/2630 (0.0%)	0.87	1/3563 (0.0%)
1	B	0.90	0/2633	0.93	2/3569 (0.1%)
All	All	0.88	1/5263 (0.0%)	0.90	3/7132 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	GLU	CD-OE2	5.14	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	301	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	200	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	171	ARG	NE-CZ-NH1	5.13	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2570	0	2588	17	0
1	B	2572	0	2569	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	25	0	16	1	0
3	A	48	0	25	2	0
3	B	48	0	25	3	0
4	A	8	0	12	0	0
4	B	12	0	18	5	0
5	A	10	0	4	0	0
6	B	5	0	0	0	0
7	A	164	0	0	6	0
7	B	168	0	0	1	0
All	All	5630	0	5257	32	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 32 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:8:VAL:HG11	7:A:661:HOH:O	1.67	0.90
1:B:142:VAL:H	4:B:504:EDO:H12	1.58	0.68
1:A:4:LYS:N	7:A:584:HOH:O	2.29	0.66
1:B:316:ASN:OD1	4:B:504:EDO:H21	2.01	0.60
1:B:142:VAL:H	4:B:504:EDO:C1	2.16	0.58

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	319/331 (96%)	311 (98%)	8 (2%)	0	100	100
1	B	321/331 (97%)	312 (97%)	9 (3%)	0	100	100
All	All	640/662 (97%)	623 (97%)	17 (3%)	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	281/293 (96%)	279 (99%)	2 (1%)	87 78
1	B	281/293 (96%)	276 (98%)	5 (2%)	64 45
All	All	562/586 (96%)	555 (99%)	7 (1%)	73 61

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	222	HIS
1	B	320	SER
1	B	275	GLN
1	A	216	TYR
1	B	302	ASN

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 (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	$\#\|Z\| > 2$
2	SUZ	A	401	-	24,27,27	1.99	6 (25%)	30,39,39	1.93	5 (16%)
3	NAP	A	402	-	44,52,52	2.18	12 (27%)	51,80,80	1.91	9 (17%)
4	EDO	A	403	-	3,3,3	0.79	0	2,2,2	0.56	0
4	EDO	A	404	-	3,3,3	0.72	0	2,2,2	0.27	0
5	TLA	A	405	-	3,9,9	0.47	0	6,12,12	1.15	0
3	NAP	B	501	-	44,52,52	2.09	10 (22%)	51,80,80	2.60	10 (19%)
4	EDO	B	502	-	3,3,3	0.58	0	2,2,2	0.39	0
4	EDO	B	503	-	3,3,3	0.78	0	2,2,2	0.22	0
4	EDO	B	504	-	3,3,3	0.44	0	2,2,2	0.28	0
6	PO4	B	505	-	4,4,4	0.58	0	6,6,6	0.67	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	SUZ	A	401	-	-	0/10/28/28	0/3/3/3
3	NAP	A	402	-	-	0/27/67/67	0/5/5/5
4	EDO	A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	A	404	-	-	0/1/1/1	0/0/0/0
5	TLA	A	405	-	-	0/4/12/12	0/0/0/0
3	NAP	B	501	-	-	0/27/67/67	0/5/5/5
4	EDO	B	502	-	-	0/1/1/1	0/0/0/0
4	EDO	B	503	-	-	0/1/1/1	0/0/0/0
4	EDO	B	504	-	-	0/1/1/1	0/0/0/0
6	PO4	B	505	-	-	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)
3	A	402	NAP	C3N-C7N	-6.14	1.41	1.50
3	B	501	NAP	C3N-C7N	-5.79	1.41	1.50
2	A	401	SUZ	C13-C10	-5.50	1.34	1.44
2	A	401	SUZ	C18-C7	-3.91	1.38	1.45
2	A	401	SUZ	C5-C6	-3.40	1.39	1.46

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	NAP	N3A-C2A-N1A	-13.88	116.77	128.86
3	A	402	NAP	N3A-C2A-N1A	-9.25	120.80	128.86
3	B	501	NAP	O2A-PA-O5B	-5.81	80.72	108.14
2	A	401	SUZ	C5-C6-C7	-4.76	120.16	129.74
3	B	501	NAP	C4D-O4D-C1D	-4.47	105.02	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SUZ	1	0
3	A	402	NAP	2	0
3	B	501	NAP	3	0
4	B	504	EDO	5	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, 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	316/331 (95%)	0.09	14 (4%) 35 42	21, 33, 50, 71	13 (4%)
1	B	318/331 (96%)	0.31	39 (12%) 5 6	17, 31, 68, 88	8 (2%)
All	All	634/662 (95%)	0.20	53 (8%) 12 15	17, 32, 60, 88	21 (3%)

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ALA	5.7
1	B	226	PRO	4.7
1	B	27	ALA	4.7
1	B	29	VAL	4.6
1	B	320	SER	4.2

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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
5	TLA	A	405	10/10	0.86	0.14	4.16	43,51,57,67	0
4	EDO	B	503	4/4	0.83	0.18	3.07	38,45,47,50	0
2	SUZ	A	401	25/25	0.84	0.16	2.58	28,39,61,65	25
4	EDO	B	502	4/4	0.93	0.10	1.25	34,36,36,40	0
3	NAP	B	501	48/48	0.91	0.14	0.61	28,59,76,82	0
3	NAP	A	402	48/48	0.96	0.09	0.08	25,35,43,58	0
4	EDO	A	403	4/4	0.98	0.08	-0.07	23,25,29,30	0
4	EDO	B	504	4/4	0.95	0.10	-0.32	29,37,39,40	0
6	PO4	B	505	5/5	0.96	0.19	-	55,57,65,75	5
4	EDO	A	404	4/4	0.80	0.18	-	54,56,66,73	0

6.5 Other polymers (i)

There are no such residues in this entry.