



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:32 PM GMT

PDB ID : 5CYM  
Title : HIV-1 reverse transcriptase complexed with 4-iodopyrazole  
Authors : Bauman, J.D.; Arnold, E.  
Deposited on : 2015-07-30  
Resolution : 2.10 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](mailto: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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20026982

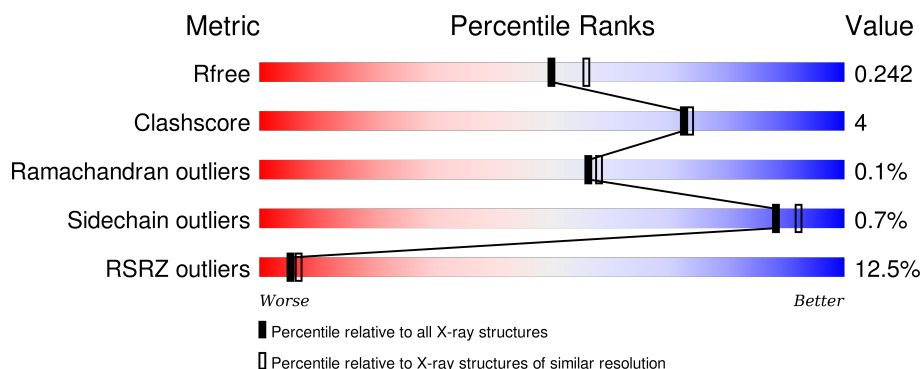
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 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	557	<div> <div>12%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
2	B	428	<div> <div>13%</div> <div>86%</div> <div>9%</div> <div>5%</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	SO4	B	501	-	-	-	X
5	EDO	A	605	-	-	-	X
5	EDO	A	606	-	-	-	X
5	EDO	B	502	-	-	-	X
5	EDO	B	503	-	-	-	X
6	IOD	A	608	-	-	-	X
6	IOD	A	613	-	-	X	-
6	IOD	A	614	-	-	X	-
6	IOD	A	615	-	-	X	-
6	IOD	A	616	-	-	X	-
7	PYZ	A	618	-	-	-	X
7	PYZ	B	509	-	-	-	X
7	PYZ	B	510	-	-	-	X
7	PYZ	B	511	-	-	-	X
8	DMS	A	619	-	-	-	X
8	DMS	B	512	-	-	-	X
8	DMS	B	513	-	-	-	X
8	DMS	B	514	-	-	-	X
8	DMS	B	515	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16183 atoms, of which 7992 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 HIV-1 reverse transcriptase, p66 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	546	Total	C	H	N	O	S	0	1	0
			8935	2878	4493	737	819	8			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

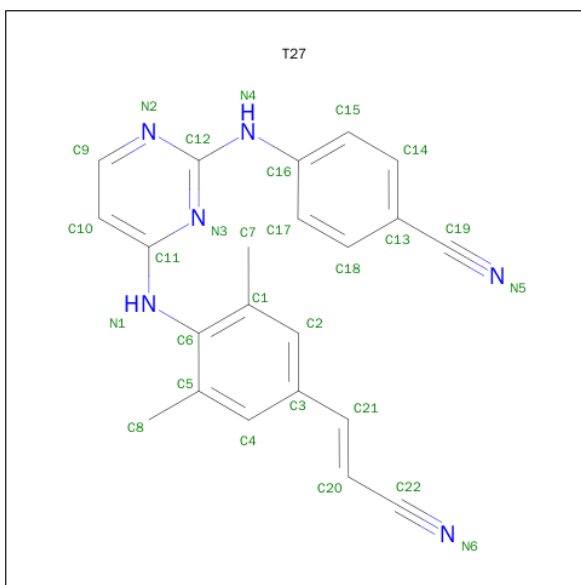
- Molecule 2 is a protein called HIV-1 reverse transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	408	Total	C	H	N	O	S	0	2	0
			6788	2201	3409	559	612	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-([4-([4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl]amino)pyrimidin-2-yl]amino)benzonitrile (three-letter code: T27) (formula: C<sub>22</sub>H<sub>18</sub>N<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			46	22	18	6		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).

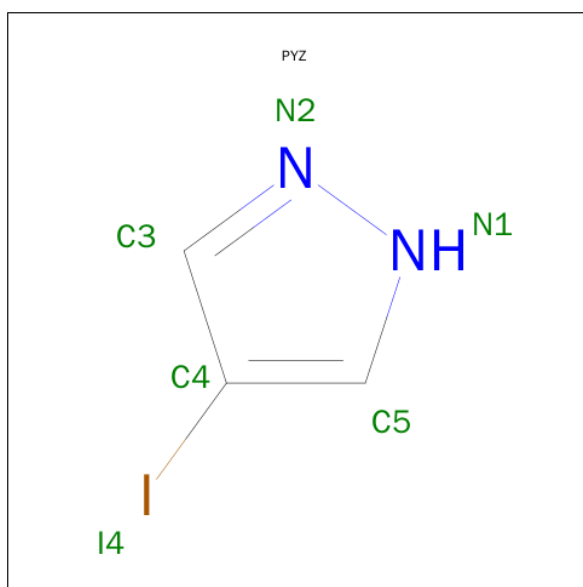


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

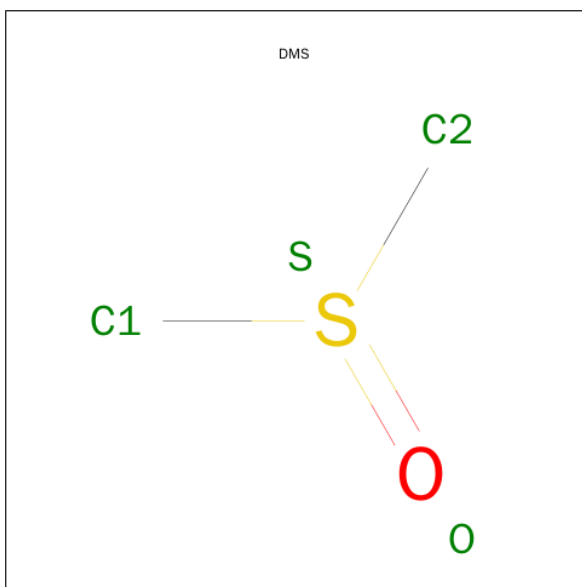
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	I	0	0
			4	4		
6	A	10	Total	I	0	0
			10	10		

- Molecule 7 is 4-IODOPYRAZOLE (three-letter code: PYZ) (formula:  $C_3H_3IN_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	A	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	B	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	B	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	B	1	Total	C	H	I	N	0	0
			9	3	3	1	2		

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

- Molecule 9 is water.

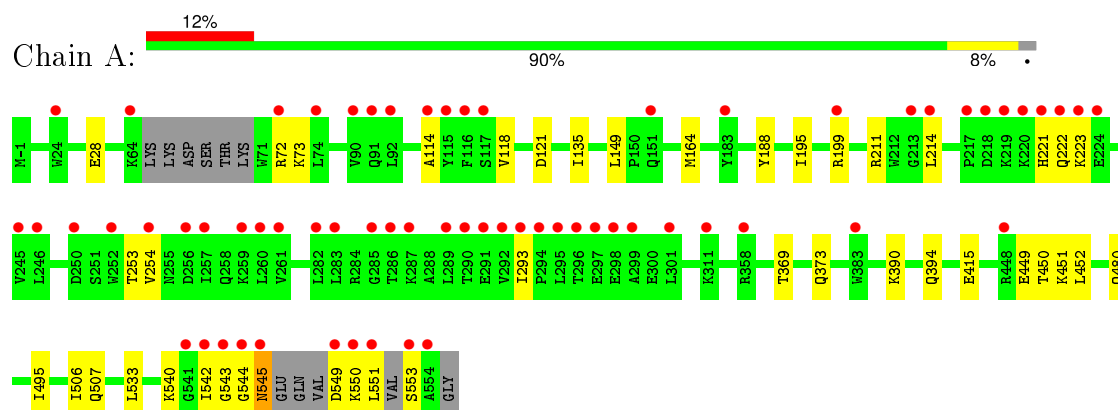
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	150	Total	O	0	0
			150	150		
9	B	86	Total	O	0	0
			86	86		



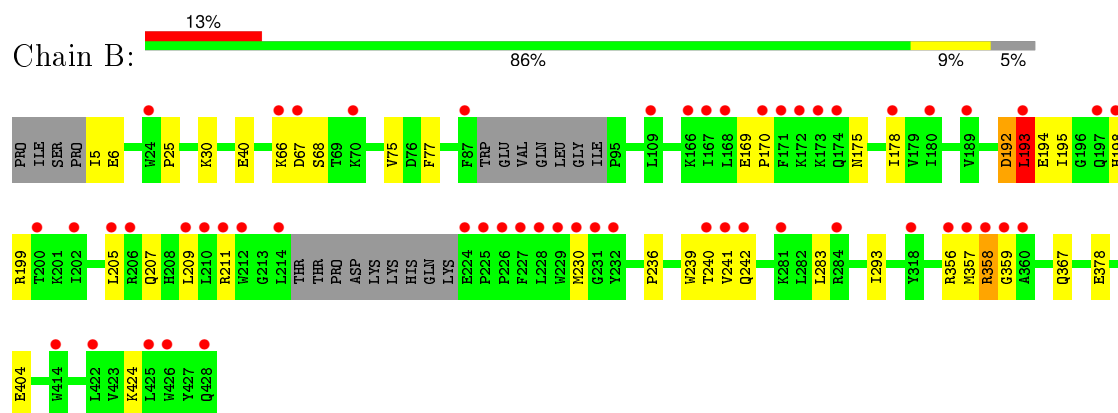
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: HIV-1 reverse transcriptase, p66 subunit



- Molecule 2: HIV-1 reverse transcriptase, p51 subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.84Å 73.48Å 109.58Å 90.00° 100.67° 90.00°	Depositor
Resolution (Å)	43.17 – 2.10 43.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.17-2.10) 98.2 (43.59-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1988)	Depositor
R, $R_{free}$	0.195 , 0.229 0.214 , 0.242	Depositor DCC
$R_{free}$ test set	3729 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 73508 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PYZ, EDO, DMS, SO4, IOD, T27

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	0.33	0/4560	0.46	0/6196
2	B	0.34	0/3484	0.51	3/4730 (0.1%)
All	All	0.34	0/8044	0.48	3/10926 (0.0%)

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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	193	LEU	CB-CG-CD2	-7.78	97.77	111.00
2	B	192	ASP	N-CA-C	-6.11	94.51	111.00
2	B	193	LEU	CA-CB-CG	5.63	128.25	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	193	LEU	Peptide

## 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	4442	4493	4490	34	0
2	B	3379	3409	3394	32	0
3	A	28	18	18	2	0
4	A	15	0	0	0	0
4	B	5	0	0	1	0
5	A	8	12	12	0	0
5	B	8	12	12	0	0
6	A	10	0	0	9	0
6	B	4	0	0	0	0
7	A	12	6	6	0	0
7	B	24	12	12	1	0
8	A	4	6	6	0	0
8	B	16	24	24	1	0
9	A	150	0	0	4	0
9	B	86	0	0	3	0
All	All	8191	7992	7974	67	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 4.

The worst 5 of 67 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)
2:B:192:ASP:O	2:B:193:LEU:HB2	1.76	0.84
1:A:543:GLY:N	2:B:283:LEU:O	2.09	0.84
6:A:614:IOD:I	6:A:615:IOD:I	3.36	0.84
1:A:394:GLN:NE2	9:A:702:HOH:O	2.16	0.79
2:B:40:GLU:OE1	9:B:601:HOH:O	2.02	0.77

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	539/557 (97%)	527 (98%)	12 (2%)	0	100	100
2	B	404/428 (94%)	392 (97%)	11 (3%)	1 (0%)	52	53
All	All	943/985 (96%)	919 (98%)	23 (2%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	193	LEU

### 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	486/495 (98%)	483 (99%)	3 (1%)	90	94
2	B	372/390 (95%)	369 (99%)	3 (1%)	86	91
All	All	858/885 (97%)	852 (99%)	6 (1%)	88	92

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	550	LYS
2	B	358	ARG
2	B	242	GLN
1	A	545	ASN
2	B	356	ARG

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](#)

Of 34 ligands modelled in this entry, 14 are monoatomic - leaving 20 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	$\# Z  > 2$
3	T27	A	601	-	30,30,30	1.17	2 (6%)	39,40,40	1.84	7 (17%)
4	SO4	A	602	-	4,4,4	0.22	0	6,6,6	0.22	0
4	SO4	A	603	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	A	604	-	4,4,4	0.26	0	6,6,6	0.10	0
5	EDO	A	605	-	3,3,3	0.45	0	2,2,2	0.33	0
5	EDO	A	606	-	3,3,3	0.50	0	2,2,2	0.34	0
7	PYZ	A	617	-	6,6,6	2.65	3 (50%)	1,7,7	0.07	0
7	PYZ	A	618	-	6,6,6	2.46	3 (50%)	1,7,7	0.29	0
8	DMS	A	619	-	3,3,3	0.63	0	3,3,3	0.65	0
4	SO4	B	501	-	4,4,4	0.23	0	6,6,6	0.12	0
5	EDO	B	502	-	3,3,3	0.43	0	2,2,2	0.35	0
5	EDO	B	503	-	3,3,3	0.42	0	2,2,2	0.31	0
7	PYZ	B	508	-	6,6,6	2.41	3 (50%)	1,7,7	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PYZ	B	509	-	6,6,6	2.41	3 (50%)	1,7,7	0.52	0
7	PYZ	B	510	-	6,6,6	2.39	3 (50%)	1,7,7	0.31	0
7	PYZ	B	511	-	6,6,6	2.40	3 (50%)	1,7,7	0.38	0
8	DMS	B	512	-	3,3,3	0.69	0	3,3,3	0.51	0
8	DMS	B	513	-	3,3,3	0.64	0	3,3,3	0.45	0
8	DMS	B	514	-	3,3,3	0.67	0	3,3,3	0.48	0
8	DMS	B	515	-	3,3,3	0.63	0	3,3,3	0.48	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
3	T27	A	601	-	-	0/13/14/14	0/3/3/3
4	SO4	A	602	-	-	0/0/0/0	0/0/0/0
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0
4	SO4	A	604	-	-	0/0/0/0	0/0/0/0
5	EDO	A	605	-	-	0/1/1/1	0/0/0/0
5	EDO	A	606	-	-	0/1/1/1	0/0/0/0
7	PYZ	A	617	-	-	0/0/0/0	0/1/1/1
7	PYZ	A	618	-	-	0/0/0/0	0/1/1/1
8	DMS	A	619	-	-	0/0/0/0	0/0/0/0
4	SO4	B	501	-	-	0/0/0/0	0/0/0/0
5	EDO	B	502	-	-	0/1/1/1	0/0/0/0
5	EDO	B	503	-	-	0/1/1/1	0/0/0/0
7	PYZ	B	508	-	-	0/0/0/0	0/1/1/1
7	PYZ	B	509	-	-	0/0/0/0	0/1/1/1
7	PYZ	B	510	-	-	0/0/0/0	0/1/1/1
7	PYZ	B	511	-	-	0/0/0/0	0/1/1/1
8	DMS	B	512	-	-	0/0/0/0	0/0/0/0
8	DMS	B	513	-	-	0/0/0/0	0/0/0/0
8	DMS	B	514	-	-	0/0/0/0	0/0/0/0
8	DMS	B	515	-	-	0/0/0/0	0/0/0/0

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	617	PYZ	C4-I4	-3.16	2.01	2.10
7	B	509	PYZ	C4-I4	-2.17	2.04	2.10
7	B	511	PYZ	C4-I4	-2.15	2.04	2.10
7	B	510	PYZ	C5-N1	2.04	1.38	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	508	PYZ	C5-N1	2.04	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	T27	C10-C9-N2	-4.38	118.74	123.88
3	A	601	T27	N2-C12-N3	-4.26	122.12	126.66
3	A	601	T27	C10-C11-N3	-2.67	118.40	123.22
3	A	601	T27	C6-N1-C11	-2.57	120.36	124.35
3	A	601	T27	C3-C4-C5	-2.46	119.46	122.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	T27	2	0
4	B	501	SO4	1	0
7	B	511	PYZ	1	0
8	B	515	DMS	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	546/557 (98%)	0.76	65 (11%) <b>6</b> <b>8</b>	32, 56, 110, 174	0
2	B	408/428 (95%)	0.93	54 (13%) <b>4</b> <b>6</b>	36, 60, 114, 154	0
All	All	954/985 (96%)	0.83	119 (12%) <b>5</b> <b>7</b>	32, 58, 112, 174	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	11.6
1	A	219	LYS	6.4
1	A	114	ALA	6.4
1	A	116	PHE	6.3
2	B	241	VAL	6.2

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	EDO	B	502	4/4	0.91	0.40	19.41	67,80,97,113	0
8	DMS	B	515	4/4	0.54	0.46	12.13	118,142,143,143	0
8	DMS	B	513	4/4	0.92	0.34	9.83	132,167,168,168	0
7	PYZ	B	510	6/6	0.82	0.40	9.07	136,146,173,176	0
7	PYZ	B	509	6/6	0.67	0.36	7.80	89,102,129,326	0
8	DMS	A	619	4/4	0.82	0.26	6.47	93,112,120,120	0
8	DMS	B	512	4/4	0.90	0.26	4.59	88,106,107,107	0
7	PYZ	A	618	6/6	0.47	0.27	4.08	112,119,144,258	0
5	EDO	A	605	4/4	0.97	0.19	3.90	57,72,80,96	0
5	EDO	B	503	4/4	0.92	0.22	3.22	54,66,88,97	0
5	EDO	A	606	4/4	0.81	0.31	3.12	67,87,109,109	0
7	PYZ	B	511	6/6	0.87	0.26	2.43	93,101,121,172	0
6	IOD	A	608	1/1	0.97	0.16	2.25	162,162,162,162	0
8	DMS	B	514	4/4	0.72	0.33	2.25	119,148,148,148	0
4	SO4	B	501	5/5	0.93	0.21	2.04	122,123,126,130	0
6	IOD	A	611	1/1	-0.11	0.36	1.09	389,389,389,389	0
3	T27	A	601	28/28	0.95	0.17	1.07	34,45,63,68	0
4	SO4	A	604	5/5	0.81	0.18	0.40	133,134,136,139	0
6	IOD	A	614	1/1	-0.05	0.18	-0.07	198,198,198,198	0
7	PYZ	B	508	6/6	0.95	0.15	-0.44	97,98,117,118	0
6	IOD	A	609	1/1	0.62	0.14	-0.52	153,153,153,153	0
4	SO4	A	602	5/5	0.93	0.12	-0.54	89,95,101,103	0
7	PYZ	A	617	6/6	0.95	0.13	-0.71	47,58,74,106	0
6	IOD	A	613	1/1	0.98	0.11	-0.82	100,100,100,100	0
6	IOD	A	616	1/1	0.66	0.13	-0.85	87,87,87,87	1
6	IOD	A	610	1/1	0.75	0.09	-0.89	182,182,182,182	0
6	IOD	A	607	1/1	0.96	0.12	-1.03	132,132,132,132	0
6	IOD	A	615	1/1	0.89	0.10	-1.09	73,73,73,73	1
4	SO4	A	603	5/5	0.82	0.14	-1.15	119,121,124,135	0
6	IOD	B	506	1/1	0.68	0.12	-1.28	216,216,216,216	0
6	IOD	B	504	1/1	0.93	0.08	-1.50	112,112,112,112	0
6	IOD	B	507	1/1	0.73	0.14	-1.57	198,198,198,198	0
6	IOD	B	505	1/1	0.88	0.07	-	160,160,160,160	0
6	IOD	A	612	1/1	0.78	0.13	-	229,229,229,229	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.