



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2025 – 07:09 pm BST

PDB ID : 9G6U / pdb\_00009g6u  
Title : p53-Y220C Core Domain Covalently Bound to 3,5-Dichloro-6-Ethylpyrazine-2-carbonitrile Soaked at 5 mM  
Authors : Stahlecker, J.; Klett, T.; Stehle, T.; Boeckler, F.M.  
Deposited on : 2024-07-19  
Resolution : 1.64 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

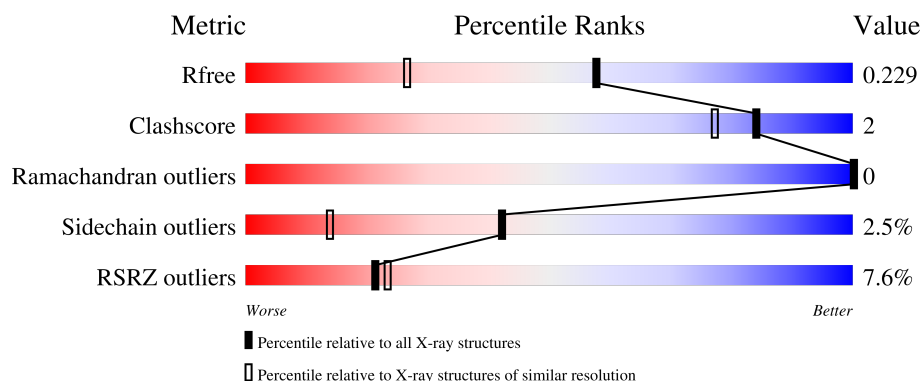
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.64 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))
$R_{free}$	164625	1015 (1.64-1.64)
Clashscore	180529	1093 (1.64-1.64)
Ramachandran outliers	177936	1077 (1.64-1.64)
Sidechain outliers	177891	1077 (1.64-1.64)
RSRZ outliers	164620	1015 (1.64-1.64)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	219	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	219	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3629 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.

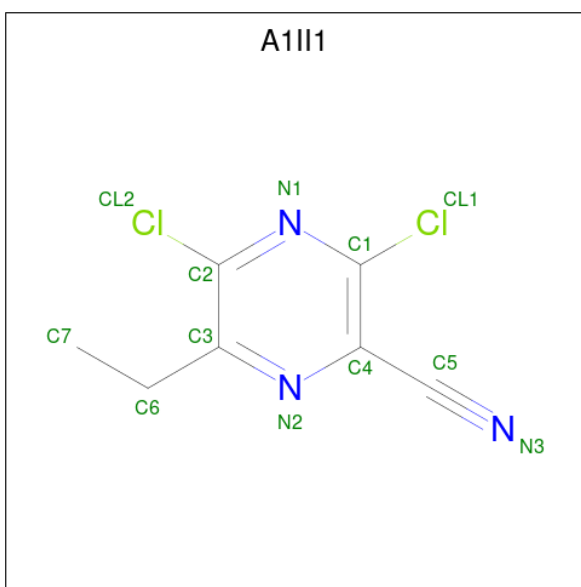
- Molecule 1 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	5	0
			1533	948	274	295	16			
1	B	198	Total	C	N	O	S	0	10	0
			1577	975	280	304	18			

There are 10 discrepancies between the modelled and reference sequences:

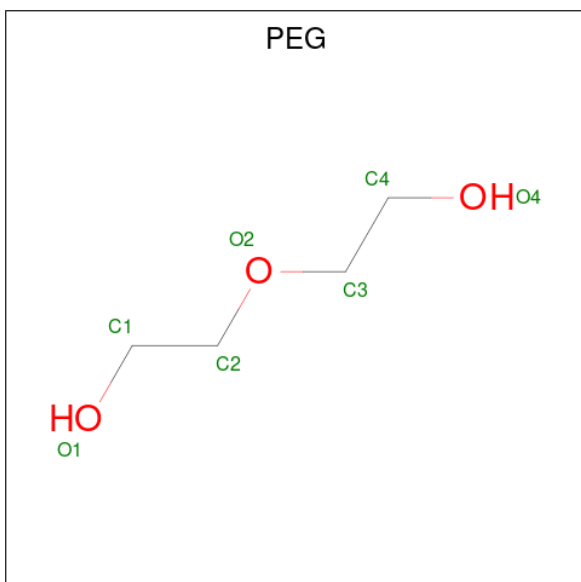
Chain	Residue	Modelled	Actual	Comment	Reference
A	133	LEU	MET	engineered mutation	UNP P04637
A	203	ALA	VAL	engineered mutation	UNP P04637
A	220	CYS	TYR	engineered mutation	UNP P04637
A	239	TYR	ASN	engineered mutation	UNP P04637
A	268	ASP	ASN	engineered mutation	UNP P04637
B	133	LEU	MET	engineered mutation	UNP P04637
B	203	ALA	VAL	engineered mutation	UNP P04637
B	220	CYS	TYR	engineered mutation	UNP P04637
B	239	TYR	ASN	engineered mutation	UNP P04637
B	268	ASP	ASN	engineered mutation	UNP P04637

- Molecule 2 is 3,5-bis(chloranyl)-6-ethyl-pyrazine-2-carbonitrile (CCD ID: A1II1) (formula:  $C_7H_5Cl_2N_3$ ).



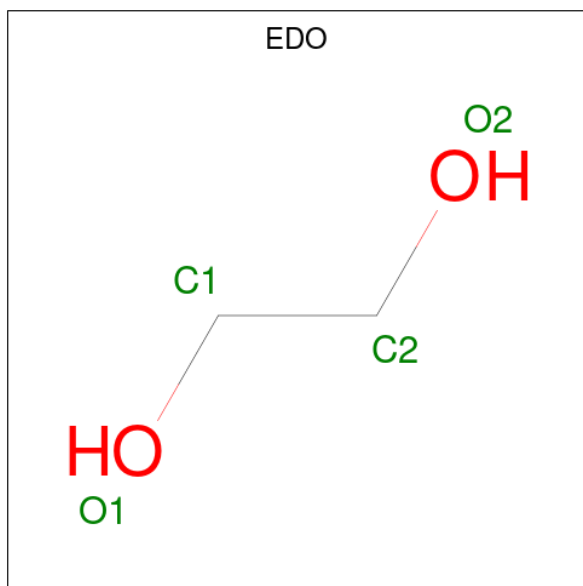
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			11	7	1	3		
2	A	1	Total	C	Cl	N	0	0
			9	6	1	2		
2	B	1	Total	C	Cl	N	0	0
			11	7	1	3		
2	B	1	Total	C	Cl	N	0	0
			10	6	1	3		
2	B	1	Total	C	N		0	0
			6	4	2			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



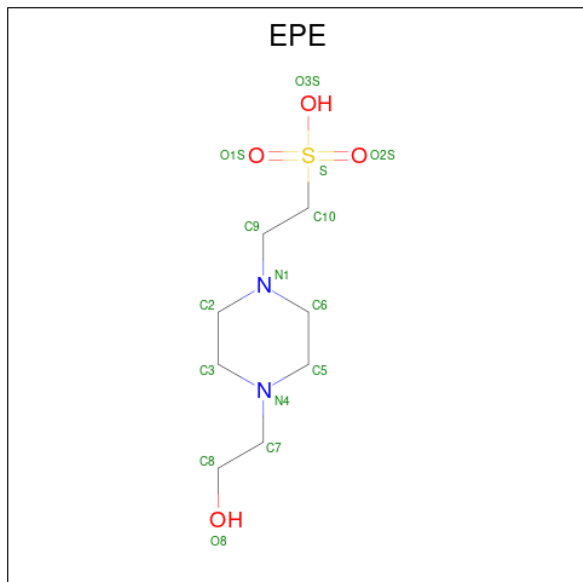
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
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 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			9	4	1	3	1		
5	A	1	Total	C	N	O	S	0	0
			9	4	1	3	1		
5	B	1	Total	C	O	S		0	0
			5	1	3	1			

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

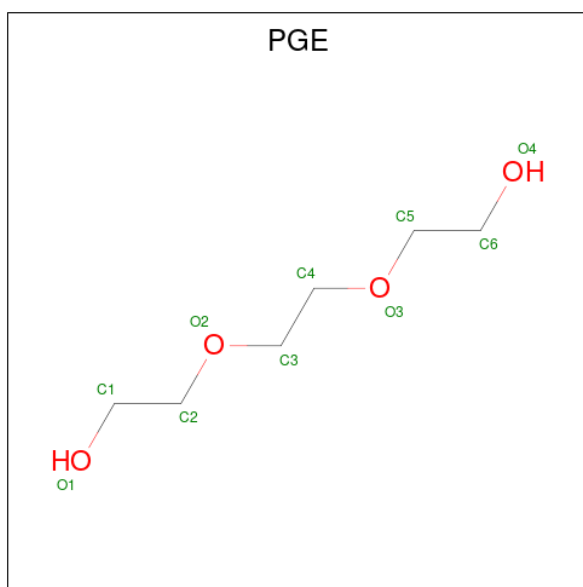
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 9 is water.

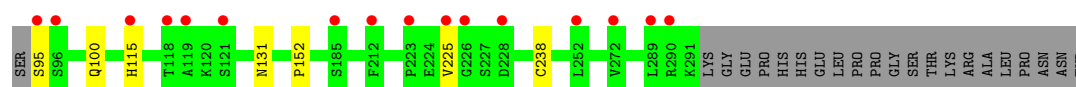
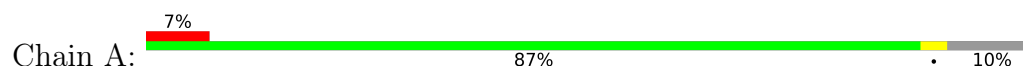
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	171	Total 171	O 171	0	0
9	B	196	Total 196	O 196	0	0



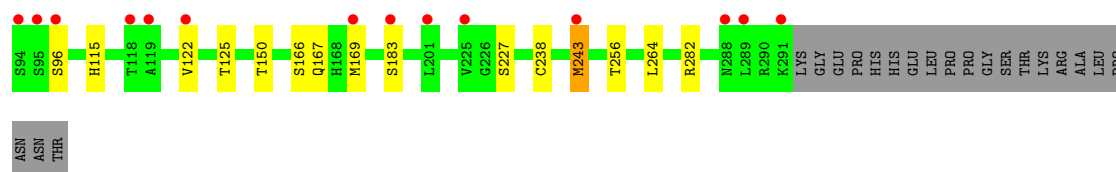
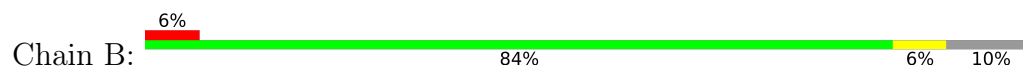
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.82Å 71.16Å 105.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 1.64 47.92 – 1.64	Depositor EDS
% Data completeness (in resolution range)	95.9 (47.92-1.64) 96.1 (47.92-1.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 1.64Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.194 , 0.229 0.194 , 0.229	Depositor DCC
$R_{free}$ test set	1501 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7856e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 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: PEG, GOL, ZN, A1II1, EPE, PGE, EDO

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	0.45	0/1569	0.62	0/2135
1	B	0.46	0/1612	0.61	0/2191
All	All	0.46	0/3181	0.61	0/4326

There are no bond length outliers.

There are no bond angle outliers.

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	1533	0	1437	5	0
1	B	1577	0	1473	8	0
2	A	20	0	0	1	0
2	B	27	0	0	1	0
3	A	12	0	15	2	0
3	B	5	0	5	0	0
4	A	24	0	36	2	0
4	B	12	0	18	0	0
5	A	18	0	8	0	0
5	B	5	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	B	18	0	24	0	0
8	B	9	0	11	3	0
9	A	171	0	0	2	0
9	B	196	0	0	1	0
All	All	3629	0	3027	14	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 2.

All (14) 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:A:412:A1II1:CL1	9:A:647:HOH:O	2.44	0.72
1:B:166[A]:SER:HA	1:B:169[A]:MET:HE3	1.76	0.66
1:A:115:HIS:HB3	3:A:405:PEG:H32	1.79	0.64
1:B:115:HIS:HB3	8:B:406:PGE:H5	1.83	0.60
1:A:95:SER:N	9:A:505:HOH:O	2.38	0.56
1:A:100:GLN:HG2	4:A:409:EDO:H12	1.89	0.55
1:A:152:PRO:HA	4:A:406:EDO:H12	1.92	0.51
1:B:150:THR:HG23	2:B:401:A1II1:N3	2.31	0.44
1:B:256[B]:THR:HG23	1:B:264:LEU:HD12	1.99	0.44
1:B:282:ARG:HH22	8:B:406:PGE:H6	1.83	0.43
1:B:122:VAL:HG11	1:B:125:THR:HB	2.00	0.42
1:A:131:ASN:HB3	3:A:402:PEG:H11	2.01	0.41
1:B:243[B]:MET:HG2	9:B:645:HOH:O	2.21	0.41
1:B:282:ARG:HH12	8:B:406:PGE:C6	2.35	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	201/219 (92%)	201 (100%)	0	0	100	100
1	B	206/219 (94%)	204 (99%)	2 (1%)	0	100	100
All	All	407/438 (93%)	405 (100%)	2 (0%)	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	169/195 (87%)	167 (99%)	2 (1%)	67	45
1	B	173/195 (89%)	164 (95%)	9 (5%)	19	2
All	All	342/390 (88%)	331 (97%)	11 (3%)	42	9

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	VAL
1	A	238	CYS
1	B	96[A]	SER
1	B	96[B]	SER
1	B	167[A]	GLN
1	B	167[B]	GLN
1	B	183	SER
1	B	227	SER
1	B	238	CYS
1	B	243[A]	MET
1	B	243[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	233	HIS

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Mol	Chain	Res	Type
1	A	235	ASN
1	B	247	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	PEG	A	402	-	6,6,6	0.16	0	5,5,5	0.21	0
5	EPE	A	404	-	8,8,15	1.08	1 (12%)	10,11,20	1.49	1 (10%)
4	EDO	B	412	-	3,3,3	0.45	0	2,2,2	0.59	0
4	EDO	A	410	-	3,3,3	0.38	0	2,2,2	0.30	0
4	EDO	A	411	-	3,3,3	0.49	0	2,2,2	0.45	0
8	PGE	B	406	-	8,8,9	0.36	0	7,7,8	0.37	0
3	PEG	A	405	-	4,4,6	0.28	0	3,3,5	0.19	0
2	A1II1	B	401	1	10,11,12	0.39	0	9,14,16	0.76	0
4	EDO	A	403	-	3,3,3	0.49	0	2,2,2	0.89	0
2	A1II1	A	401	1	10,11,12	0.41	0	9,14,16	1.00	0
7	GOL	B	404	-	5,5,5	0.72	0	5,5,5	0.94	0
4	EDO	A	409	-	3,3,3	0.46	0	2,2,2	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	B	411	-	5,5,5	0.72	0	5,5,5	1.06	0
4	EDO	A	407	-	3,3,3	0.54	0	2,2,2	0.09	0
4	EDO	B	410	-	3,3,3	0.48	0	2,2,2	0.18	0
2	A1II1	A	412	1	9,9,12	1.11	1 (11%)	10,12,16	0.65	0
3	PEG	B	403	-	4,4,6	0.33	0	3,3,5	0.25	0
7	GOL	B	407	-	5,5,5	0.94	0	5,5,5	1.22	1 (20%)
4	EDO	A	406	-	3,3,3	0.48	0	2,2,2	0.30	0
4	EDO	B	405	-	3,3,3	0.48	0	2,2,2	0.21	0
5	EPE	B	408	-	4,4,15	1.02	0	5,6,20	1.44	1 (20%)
2	A1II1	B	409	1	6,6,12	0.35	0	6,6,16	0.74	0
2	A1II1	B	402	1	9,10,12	0.52	0	10,13,16	0.94	0
5	EPE	A	408	-	8,8,15	1.16	1 (12%)	10,11,20	1.57	2 (20%)

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	PEG	A	402	-	-	3/4/4/4	-
5	EPE	A	404	-	-	2/6/6/19	-
4	EDO	B	412	-	-	1/1/1/1	-
4	EDO	A	410	-	-	1/1/1/1	-
4	EDO	A	411	-	-	0/1/1/1	-
8	PGE	B	406	-	-	4/6/6/7	-
3	PEG	A	405	-	-	2/2/2/4	-
2	A1II1	B	401	1	-	1/2/4/4	0/1/1/1
4	EDO	A	403	-	-	1/1/1/1	-
7	GOL	B	404	-	-	2/4/4/4	-
2	A1II1	A	401	1	-	0/2/4/4	0/1/1/1
4	EDO	A	409	-	-	1/1/1/1	-
7	GOL	B	411	-	-	3/4/4/4	-
4	EDO	A	407	-	-	0/1/1/1	-
4	EDO	B	410	-	-	1/1/1/1	-
2	A1II1	A	412	1	-	-	0/1/1/1
3	PEG	B	403	-	-	1/2/2/4	-
7	GOL	B	407	-	-	3/4/4/4	-
4	EDO	A	406	-	-	0/1/1/1	-
4	EDO	B	405	-	-	0/1/1/1	-
2	A1II1	B	409	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1II1	B	402	1	-	0/0/2/4	0/1/1/1
5	EPE	A	408	-	-	6/6/6/19	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	408	EPE	C10-S	3.06	1.81	1.77
2	A	412	A1II1	C5-C4	-2.90	1.45	1.50
5	A	404	EPE	C10-S	2.72	1.81	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404	EPE	O1S-S-C10	3.74	111.42	106.92
5	A	408	EPE	O3S-S-C10	3.34	111.17	105.77
5	A	408	EPE	O1S-S-C10	3.15	110.70	106.92
5	B	408	EPE	O2S-S-O1S	-3.00	109.92	118.02
7	B	407	GOL	C3-C2-C1	-2.11	103.51	111.70

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	EPE	C10-C9-N1-C6
5	A	408	EPE	C10-C9-N1-C6
5	A	408	EPE	S-C10-C9-N1
7	B	404	GOL	O1-C1-C2-C3
7	B	407	GOL	O1-C1-C2-C3
7	B	411	GOL	C1-C2-C3-O3
7	B	407	GOL	O1-C1-C2-O2
3	A	405	PEG	O2-C3-C4-O4
3	A	402	PEG	O2-C3-C4-O4
7	B	404	GOL	O1-C1-C2-O2
4	A	403	EDO	O1-C1-C2-O2
3	A	402	PEG	O1-C1-C2-O2
8	B	406	PGE	O3-C5-C6-O4
8	B	406	PGE	C1-C2-O2-C3
3	B	403	PEG	C4-C3-O2-C2
7	B	407	GOL	O2-C2-C3-O3
4	A	409	EDO	O1-C1-C2-O2
5	A	404	EPE	C10-C9-N1-C2

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Mol	Chain	Res	Type	Atoms
5	A	408	EPE	C10-C9-N1-C2
2	B	401	A1II1	N2-C3-C6-C7
3	A	405	PEG	C4-C3-O2-C2
7	B	411	GOL	O1-C1-C2-O2
7	B	411	GOL	O2-C2-C3-O3
8	B	406	PGE	C6-C5-O3-C4
5	A	408	EPE	C9-C10-S-O3S
4	A	410	EDO	O1-C1-C2-O2
4	B	410	EDO	O1-C1-C2-O2
5	A	408	EPE	C9-C10-S-O1S
5	A	408	EPE	C9-C10-S-O2S
3	A	402	PEG	C1-C2-O2-C3
4	B	412	EDO	O1-C1-C2-O2
8	B	406	PGE	O2-C3-C4-O3

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	PEG	1	0
8	B	406	PGE	3	0
3	A	405	PEG	1	0
2	B	401	A1II1	1	0
4	A	409	EDO	1	0
2	A	412	A1II1	1	0
4	A	406	EDO	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

### 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<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	197/219 (89%)	0.83	16 (8%) 19 20	11, 31, 57, 71	5 (2%)
1	B	198/219 (90%)	0.76	14 (7%) 23 25	12, 30, 55, 73	10 (5%)
All	All	395/438 (90%)	0.80	30 (7%) 21 23	11, 31, 56, 73	15 (3%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	SER	4.8
1	A	225	VAL	4.6
1	A	119	ALA	4.3
1	B	225	VAL	4.0
1	B	96[A]	SER	3.6
1	B	119	ALA	3.4
1	A	226	GLY	3.4
1	A	118	THR	3.3
1	A	228	ASP	2.9
1	A	252	LEU	2.8
1	A	115	HIS	2.8
1	B	201	LEU	2.7
1	B	95	SER	2.6
1	B	183	SER	2.6
1	B	243[A]	MET	2.6
1	A	185	SER	2.5
1	B	288	ASN	2.5
1	A	290	ARG	2.4
1	B	122	VAL	2.4
1	B	169[A]	MET	2.3
1	A	95	SER	2.3
1	A	96	SER	2.2
1	A	272	VAL	2.2
1	A	212	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	291	LYS	2.1
1	A	223	PRO	2.1
1	B	289	LEU	2.1
1	B	118	THR	2.0
1	A	121	SER	2.0
1	A	289	LEU	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	A1II1	B	409	6/12	0.61	0.18	54,60,66,68	0
4	EDO	A	407	4/4	0.61	0.18	53,55,57,60	0
2	A1II1	A	412	9/12	0.63	0.15	54,60,69,102	0
3	PEG	A	405	5/7	0.68	0.20	47,49,56,60	0
4	EDO	A	403	4/4	0.71	0.19	49,50,51,64	0
5	EPE	A	404	9/15	0.71	0.19	50,59,73,84	0
5	EPE	B	408	5/15	0.71	0.16	61,64,73,89	0
4	EDO	B	412	4/4	0.72	0.19	50,52,55,58	0
7	GOL	B	404	6/6	0.72	0.18	43,51,52,53	0
2	A1II1	B	402	10/12	0.74	0.15	48,53,58,76	0
4	EDO	B	410	4/4	0.75	0.15	44,46,51,56	0
5	EPE	A	408	9/15	0.75	0.17	45,50,65,69	0
4	EDO	A	411	4/4	0.76	0.14	47,48,52,62	0
4	EDO	B	405	4/4	0.76	0.23	42,49,52,56	0
3	PEG	A	402	7/7	0.77	0.17	40,46,51,51	0
7	GOL	B	411	6/6	0.77	0.13	49,57,59,61	0
3	PEG	B	403	5/7	0.80	0.16	41,44,50,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	B	407	6/6	0.81	0.17	45,48,49,61	0
4	EDO	A	406	4/4	0.82	0.16	45,48,50,55	0
4	EDO	A	410	4/4	0.82	0.14	43,48,55,57	0
8	PGE	B	406	9/10	0.82	0.15	41,44,53,57	0
4	EDO	A	409	4/4	0.83	0.15	35,40,47,47	0
2	A1II1	B	401	11/12	0.90	0.11	33,40,54,60	0
2	A1II1	A	401	11/12	0.93	0.12	35,39,50,52	0
6	ZN	B	413	1/1	0.98	0.03	27,27,27,27	0
6	ZN	A	413	1/1	0.99	0.04	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.