



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:05 AM BST

PDB ID : 5KSH  
Title : Crystal structure of penicillin-binding protein 2 from *Neisseria gonorrhoeae* containing an A501T mutation associated with cephalosporin resistance  
Authors : Fedarovich, A.; Davies, C.  
Deposited on : 2016-07-08  
Resolution : 2.40 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

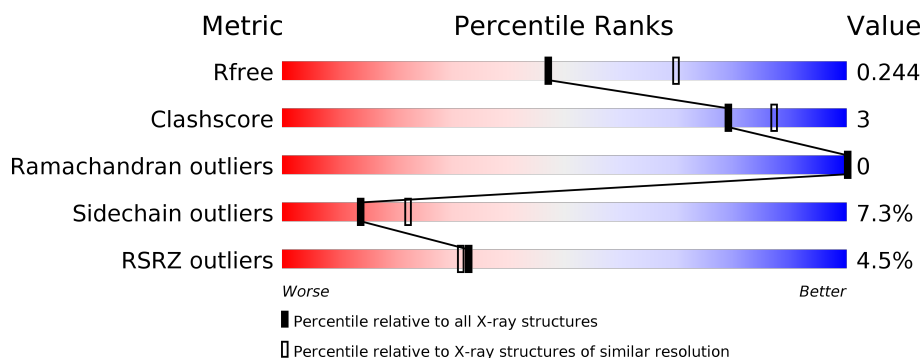
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	540	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>10%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	540	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>9%</div> <div>•</div> <div>19%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6898 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 Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	P	S	0	1	0
			3453	2163	624	657	1	8			
1	B	436	Total	C	N	O	P	S	0	0	0
			3328	2087	597	635	1	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLY	-	expression tag	UNP P08149
A	43	SER	-	expression tag	UNP P08149
A	501	THR	ALA	engineered mutation	UNP P08149
A	504	LEU	PHE	engineered mutation	UNP P08149
A	510	VAL	ALA	engineered mutation	UNP P08149
A	516	GLY	ALA	engineered mutation	UNP P08149
A	551	SER	PRO	engineered mutation	UNP P08149
B	42	GLY	-	expression tag	UNP P08149
B	43	SER	-	expression tag	UNP P08149
B	501	THR	ALA	engineered mutation	UNP P08149
B	504	LEU	PHE	engineered mutation	UNP P08149
B	510	VAL	ALA	engineered mutation	UNP P08149
B	516	GLY	ALA	engineered mutation	UNP P08149
B	551	SER	PRO	engineered mutation	UNP P08149

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

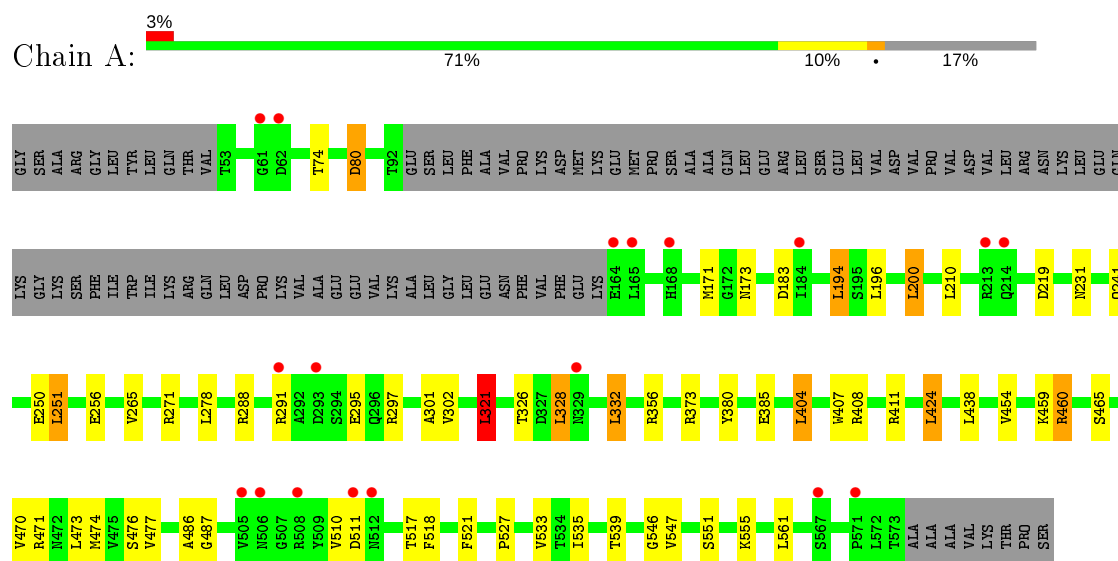
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	17	Total	O	0	0
			17	17		

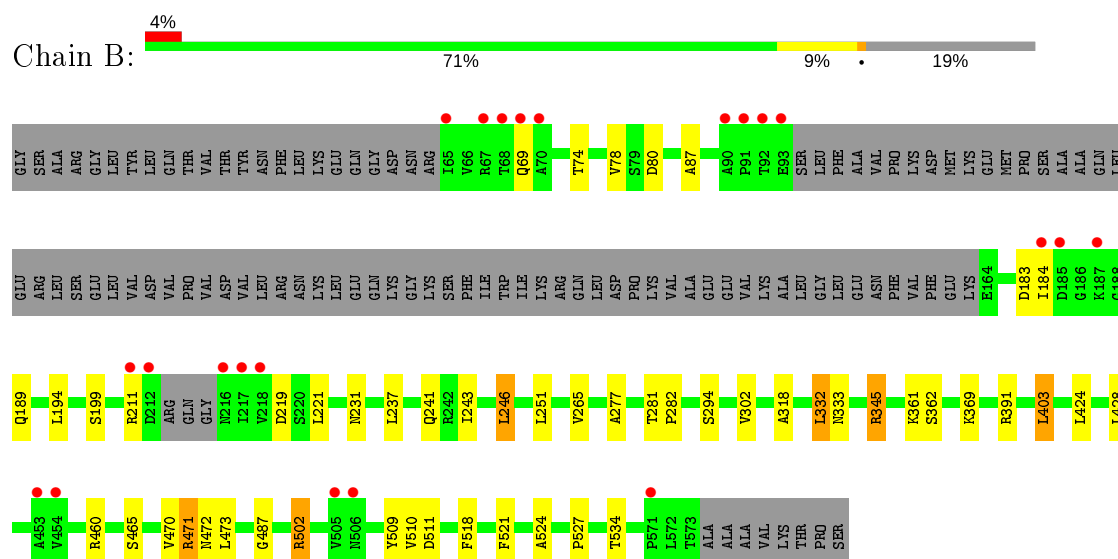
### 3 Residue-property plots [i](#)

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: Penicillin-binding protein 2



#### • Molecule 1: Penicillin-binding protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.60Å 137.20Å 229.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.11 – 2.40 46.04 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.4 (44.11-2.40) 98.5 (46.04-2.39)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.218 , 0.244 0.217 , 0.244	Depositor DCC
$R_{free}$ test set	3632 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 30.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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, 0.333 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: GOL, SO4, SEP

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	0.67	0/3512	0.90	14/4755 (0.3%)
1	B	0.63	0/3379	0.84	8/4576 (0.2%)
All	All	0.65	0/6891	0.87	22/9331 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	A	460	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	460	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	408	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	332	LEU	CA-CB-CG	7.05	131.52	115.30
1	B	345	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	332	LEU	CA-CB-CG	6.63	130.55	115.30
1	A	297	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	A	321	LEU	CA-CB-CG	6.47	130.19	115.30
1	A	171	MET	CG-SD-CE	-6.26	90.19	100.20
1	B	403	LEU	CA-CB-CG	6.11	129.36	115.30
1	A	80	ASP	CB-CG-OD1	5.87	123.59	118.30
1	A	80	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	391	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	221	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	246	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	297	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	424	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	345	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	194	LEU	CB-CG-CD2	5.15	119.76	111.00
1	B	471	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	183	ASP	CB-CG-OD2	5.07	122.86	118.30



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	3453	0	3453	20	0
1	B	3328	0	3336	18	0
2	A	6	0	8	0	0
2	B	12	0	16	0	0
3	A	25	0	0	0	0
3	B	35	0	0	0	0
4	A	22	0	0	0	0
4	B	17	0	0	0	0
All	All	6898	0	6813	38	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 (38) 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:251:LEU:HG	1:A:265:VAL:HG23	1.71	0.72
1:A:510:VAL:HG12	1:A:511:ASP:H	1.59	0.67
1:A:74:THR:H	1:A:231:ASN:ND2	1.93	0.66
1:A:328:LEU:HD22	1:A:328:LEU:H	1.69	0.58
1:B:183:ASP:HB3	1:B:189:GLN:NE2	2.19	0.58
1:B:183:ASP:HB3	1:B:189:GLN:HE21	1.69	0.57
1:A:380:TYR:CE2	1:A:404:LEU:HD13	2.42	0.54
1:A:438:LEU:HD13	1:A:474:MET:CE	2.40	0.51
1:B:74:THR:H	1:B:231:ASN:ND2	2.08	0.51
1:A:196:LEU:HB2	1:A:200:LEU:HD22	1.92	0.50
1:A:385:GLU:OE1	1:A:459:LYS:HE2	2.13	0.49
1:B:471:ARG:HD3	1:B:527:PRO:HG3	1.95	0.47
1:A:321:LEU:HD13	1:A:326:THR:HG23	1.96	0.47
1:B:74:THR:H	1:B:231:ASN:HD22	1.63	0.47
1:B:318:ALA:HB2	1:B:470:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:THR:OG1	1:B:282:PRO:HA	2.16	0.46
1:A:250:GLU:OE2	1:A:555:LYS:HD3	2.16	0.46
1:B:471:ARG:HD2	1:B:524:ALA:O	2.15	0.46
1:B:69:GLN:HE21	1:B:211:ARG:HE	1.63	0.45
1:A:486:ALA:HB3	1:A:546:GLY:O	2.16	0.45
1:A:471:ARG:HG2	1:A:521:PHE:CE2	2.51	0.45
1:B:78:VAL:HB	1:B:87:ALA:HB3	1.99	0.44
1:A:278:LEU:HD21	1:A:301:ALA:HB3	1.99	0.44
1:A:356:ARG:NH1	1:A:476:SER:HB3	2.33	0.44
1:B:333:ASN:O	1:B:369:LYS:NZ	2.39	0.44
1:B:471:ARG:HG2	1:B:521:PHE:CZ	2.53	0.43
1:A:265:VAL:HG22	1:A:533:VAL:HG22	2.01	0.43
1:B:243:ILE:HG22	1:B:277:ALA:HB2	2.01	0.42
1:B:487:GLY:HA3	1:B:518:PHE:CZ	2.54	0.42
1:B:471:ARG:HG2	1:B:521:PHE:CE2	2.55	0.41
1:A:474:MET:O	1:A:477:VAL:HG13	2.20	0.41
1:B:428:LEU:HD13	1:B:534:THR:HG23	2.02	0.41
1:A:471:ARG:HD3	1:A:527:PRO:CG	2.50	0.41
1:B:502:ARG:HG3	1:B:509:TYR:CG	2.55	0.41
1:A:487:GLY:HA3	1:A:518:PHE:CZ	2.56	0.41
1:A:470:VAL:HG12	1:A:474:MET:HE1	2.03	0.40
1:B:251:LEU:HD22	1:B:265:VAL:HG23	2.03	0.40
1:A:380:TYR:HB2	1:A:407:TRP:HB3	2.02	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	446/540 (83%)	439 (98%)	7 (2%)	0	100	100
1	B	429/540 (79%)	421 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	875/1080 (81%)	860 (98%)	15 (2%)	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	363/439 (83%)	333 (92%)	30 (8%)	11	17
1	B	350/439 (80%)	328 (94%)	22 (6%)	18	28
All	All	713/878 (81%)	661 (93%)	52 (7%)	14	22

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASP
1	A	173	ASN
1	A	194	LEU
1	A	200	LEU
1	A	210	LEU
1	A	219	ASP
1	A	241	GLN
1	A	251	LEU
1	A	256	GLU
1	A	271	ARG
1	A	288	ARG
1	A	291	ARG
1	A	295	GLU
1	A	302	VAL
1	A	321	LEU
1	A	328	LEU
1	A	332	LEU
1	A	373	ARG
1	A	404	LEU
1	A	411	ARG

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Mol	Chain	Res	Type
1	A	424	LEU
1	A	454	VAL
1	A	460	ARG
1	A	473	LEU
1	A	517	THR
1	A	535	ILE
1	A	539	THR
1	A	547	VAL
1	A	551	SER
1	A	561	LEU
1	B	80	ASP
1	B	184	ILE
1	B	194	LEU
1	B	199	SER
1	B	219	ASP
1	B	237	LEU
1	B	241	GLN
1	B	246	LEU
1	B	294	SER
1	B	302	VAL
1	B	332	LEU
1	B	345	ARG
1	B	361	LYS
1	B	362	SER
1	B	403	LEU
1	B	424	LEU
1	B	460	ARG
1	B	472	ASN
1	B	473	LEU
1	B	502	ARG
1	B	510	VAL
1	B	511	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	231	ASN
1	A	252	ASN
1	A	425	GLN
1	B	69	GLN
1	B	189	GLN

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Mol	Chain	Res	Type
1	B	231	ASN
1	B	252	ASN
1	B	457	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	SEP	A	465	1	8,9,10	1.16	1 (12%)	8,12,14	4.33	3 (37%)
1	SEP	B	465	1	8,9,10	1.20	1 (12%)	8,12,14	3.56	2 (25%)

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
1	SEP	A	465	1	-	2/5/8/10	-
1	SEP	B	465	1	-	2/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	465	SEP	P-OG	2.38	1.67	1.60
1	A	465	SEP	P-OG	2.23	1.67	1.60

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	SEP	OG-CB-CA	11.40	119.24	108.14
1	B	465	SEP	OG-CB-CA	8.72	116.63	108.14
1	B	465	SEP	P-OG-CB	4.54	130.81	118.30
1	A	465	SEP	P-OG-CB	3.81	128.78	118.30
1	A	465	SEP	O3P-P-O2P	2.16	115.91	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	465	SEP	N-CA-CB-OG
1	B	465	SEP	N-CA-CB-OG
1	B	465	SEP	CA-CB-OG-P
1	A	465	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 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	$\# Z  > 2$
3	SO4	A	606	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	B	606	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	A	602	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	A	604	-	4,4,4	0.36	0	6,6,6	0.13	0
3	SO4	B	605	-	4,4,4	0.26	0	6,6,6	0.19	0
2	GOL	A	601	-	5,5,5	0.18	0	5,5,5	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	607	-	4,4,4	0.32	0	6,6,6	0.10	0
2	GOL	B	601	-	5,5,5	0.23	0	5,5,5	0.53	0
3	SO4	A	603	-	4,4,4	0.36	0	6,6,6	0.22	0
3	SO4	B	603	-	4,4,4	0.36	0	6,6,6	0.13	0
2	GOL	B	602	-	5,5,5	0.35	0	5,5,5	0.47	0
3	SO4	B	609	-	4,4,4	0.38	0	6,6,6	0.13	0
3	SO4	B	604	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	B	608	-	4,4,4	0.35	0	6,6,6	0.18	0
3	SO4	A	605	-	4,4,4	0.36	0	6,6,6	0.15	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	GOL	B	601	-	-	2/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
2	GOL	B	602	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	GOL	C1-C2-C3-O3
2	B	602	GOL	C1-C2-C3-O3
2	B	601	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	449/540 (83%)	0.21	18 (4%)	38 37	33, 49, 79, 114	1 (0%)
1	B	435/540 (80%)	0.09	22 (5%)	28 26	30, 46, 80, 109	0
All	All	884/1080 (81%)	0.15	40 (4%)	33 31	30, 48, 80, 114	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	ASN	5.0
1	A	511	ASP	4.8
1	A	214	GLN	4.5
1	A	506	ASN	4.0
1	B	65	ILE	3.9
1	A	213	ARG	3.9
1	B	184	ILE	3.8
1	A	61	GLY	3.8
1	B	454	VAL	3.8
1	A	62	ASP	3.7
1	B	217	ILE	3.7
1	B	67	ARG	3.5
1	B	90	ALA	3.4
1	A	505	VAL	3.2
1	B	218	VAL	3.2
1	B	212	ASP	3.1
1	B	92	THR	3.1
1	A	184	ILE	3.0
1	B	211	ARG	2.8
1	A	164	GLU	2.6
1	B	185	ASP	2.6
1	B	68	THR	2.6
1	B	453	ALA	2.5
1	B	91	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	571	PRO	2.5
1	B	69	GLN	2.5
1	A	329	ASN	2.4
1	B	216	ASN	2.4
1	B	70	ALA	2.4
1	B	187	LYS	2.3
1	A	571	PRO	2.3
1	B	505	VAL	2.2
1	A	508	ARG	2.2
1	B	93	GLU	2.2
1	A	293	ASP	2.1
1	B	506	ASN	2.1
1	A	291	ARG	2.1
1	A	567	SER	2.1
1	A	168[A]	HIS	2.1
1	A	165	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	465	10/11	0.85	0.17	62,68,71,74	4
1	SEP	B	465	10/11	0.86	0.17	53,58,63,65	4

## 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( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	606	5/5	0.84	0.20	58,59,62,62	5
3	SO4	B	609	5/5	0.84	0.22	84,84,91,94	0
3	SO4	B	603	5/5	0.87	0.17	91,92,95,96	0
3	SO4	A	603	5/5	0.89	0.23	83,84,89,91	0
3	SO4	A	605	5/5	0.89	0.15	77,83,87,92	0
2	GOL	A	601	6/6	0.90	0.20	49,50,51,51	0
2	GOL	B	602	6/6	0.91	0.20	58,62,65,66	0
3	SO4	B	608	5/5	0.92	0.17	68,73,75,80	0
3	SO4	A	604	5/5	0.92	0.30	85,86,90,92	0
3	SO4	B	604	5/5	0.93	0.20	83,86,88,90	0
3	SO4	B	606	5/5	0.95	0.12	87,88,91,93	0
2	GOL	B	601	6/6	0.96	0.17	46,53,55,57	0
3	SO4	B	605	5/5	0.96	0.17	68,69,74,78	0
3	SO4	A	602	5/5	0.96	0.32	100,101,102,103	0
3	SO4	B	607	5/5	0.98	0.13	62,63,68,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.