



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:29 AM UTC

PDB ID : 3EQV / pdb_00003eqv
Title : Crystal structure of penicillin-binding protein 2 from *Neisseria gonorrhoeae* containing four mutations associated with penicillin resistance
Authors : Powell, A.J.; Deacon, A.M.; Nicholas, R.A.; Davies, C.
Deposited on : 2008-10-01
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

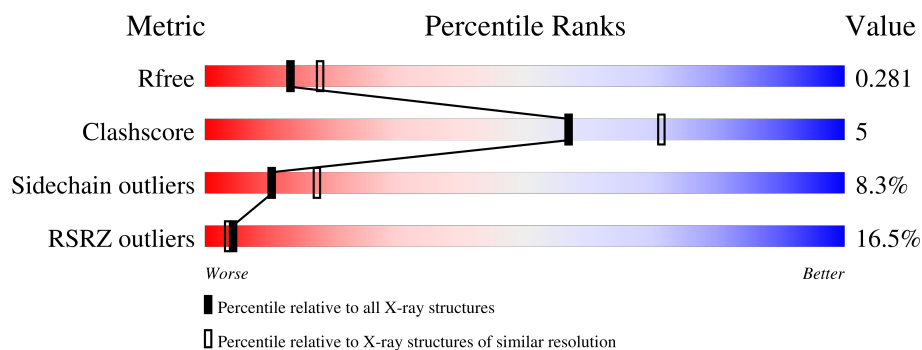
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	542	11% 69% 11% • 18%
1	B	542	16% 68% 10% • 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6805 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.

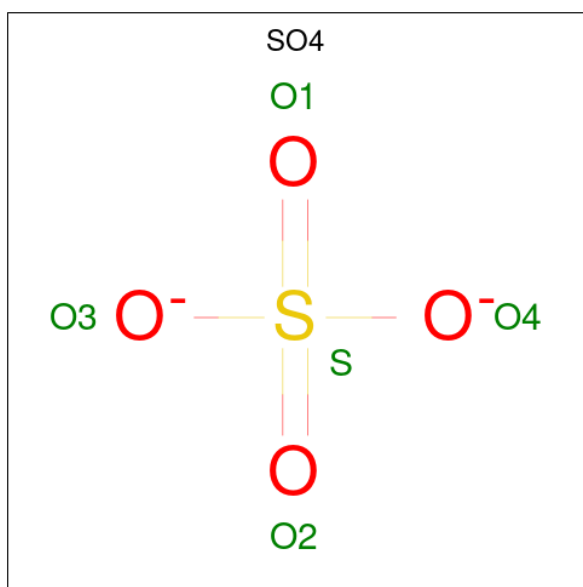
- Molecule 1 is a protein called Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	P	S	0	1	0
			3395	2126	613	647	1	8			
1	B	426	Total	C	N	O	P	S	0	0	0
			3244	2034	583	618	1	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLY	-	expression tag	UNP P08149
A	41	SER	-	expression tag	UNP P08149
A	42	GLY	-	expression tag	UNP P08149
A	43	GLY	-	expression tag	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	40	GLY	-	expression tag	UNP P08149
B	41	SER	-	expression tag	UNP P08149
B	42	GLY	-	expression tag	UNP P08149
B	43	GLY	-	expression tag	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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



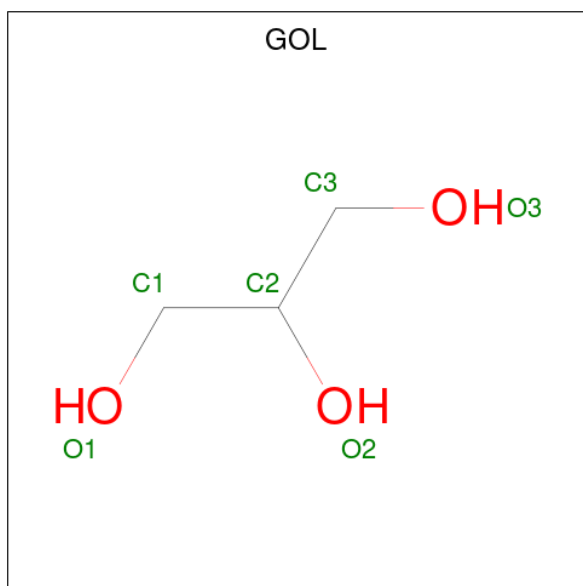
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

Continued on next page...

Continued from previous page...

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

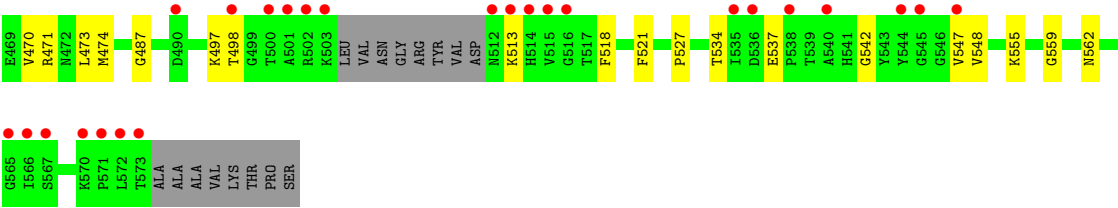
- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	39	Total	O	0	0
			39	39		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.60Å 137.20Å 229.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.10 – 2.40 48.10 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.10-2.40) 98.0 (48.10-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.253 (Not available) , 0.281	Depositor DCC
R_{free} test set	3558 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.797	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6805	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: SEP, GOL, SO4

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	0.72	2/3452 (0.1%)	0.95	1/4671 (0.0%)
1	B	0.67	0/3293	0.90	1/4457 (0.0%)
All	All	0.70	2/6745 (0.0%)	0.92	2/9128 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	ASN	CG-ND2	10.73	1.55	1.33
1	A	333	ASN	CG-OD1	5.85	1.34	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	ASN	OD1-CG-ND2	5.37	127.97	122.60
1	B	542	GLY	N-CA-C	5.33	118.26	112.29

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	3395	0	3392	35	0
1	B	3244	0	3252	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	30	0	0	0	0
2	B	45	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	40	0	0	0	0
4	B	39	0	0	0	0
All	All	6805	0	6660	62	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 5.

All (62) 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:522:ALA:HB3	1:A:557:MET:HE2	1.24	1.16
1:B:92:THR:HB	1:B:93:GLU:HA	1.49	0.94
1:A:251:LEU:HG	1:A:265:VAL:HG23	1.49	0.94
1:A:86:LEU:CD2	1:A:171:MET:HE3	1.99	0.93
1:B:438:LEU:HD13	1:B:474:MET:HE1	1.63	0.80
1:A:470:VAL:HG12	1:A:474:MET:HE2	1.63	0.79
1:A:86:LEU:HD22	1:A:171:MET:HE3	1.69	0.74
1:B:470:VAL:HG12	1:B:474:MET:HE2	1.69	0.74
1:A:86:LEU:CD2	1:A:171:MET:CE	2.65	0.73
1:B:513:LYS:HB3	1:B:537:GLU:HG2	1.73	0.68
1:A:259:GLN:HB3	1:A:539:THR:HB	1.80	0.64
1:A:171:MET:SD	1:A:241:GLN:NE2	2.72	0.63
1:B:468:ARG:HH11	1:B:468:ARG:HG3	1.64	0.62
1:A:529:VAL:HB	1:A:557:MET:HE1	1.82	0.61
1:B:318:ALA:HB2	1:B:470:VAL:HG21	1.83	0.59
1:A:438:LEU:HD13	1:A:474:MET:HE1	1.83	0.59
1:A:380:TYR:CE2	1:A:404:LEU:HD13	2.37	0.59
1:A:281:THR:HG22	1:A:282:PRO:HA	1.85	0.58
1:B:183:ASP:HB3	1:B:189:GLN:HE21	1.69	0.57
1:A:251:LEU:HG	1:A:265:VAL:CG2	2.30	0.57
1:A:53:THR:HB	1:A:58:LYS:HE3	1.87	0.56
1:A:173:ASN:C	1:A:173:ASN:HD22	2.14	0.54
1:A:557:MET:HE3	1:A:561:LEU:HD13	1.90	0.54
1:A:86:LEU:HD23	1:A:171:MET:HE3	1.87	0.54
1:B:250:GLU:OE2	1:B:555:LYS:HD3	2.09	0.53
1:B:471:ARG:HG2	1:B:521:PHE:CE2	2.44	0.53
1:A:305:MET:HG2	1:A:402:GLY:HA2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASP:HB2	1:A:296:GLN:OE1	2.11	0.51
1:A:356:ARG:NH1	1:A:476:SER:OG	2.44	0.50
1:A:557:MET:HE3	1:A:561:LEU:CD1	2.42	0.50
1:A:471:ARG:HG2	1:A:521:PHE:CE2	2.46	0.49
1:B:246:LEU:HD11	1:B:559:GLY:HA3	1.94	0.49
1:B:67:ARG:NH1	1:B:67:ARG:HB2	2.28	0.49
1:A:167:ARG:HD2	1:A:193:GLU:OE2	2.14	0.47
1:A:428:LEU:HD13	1:A:534:THR:HG23	1.97	0.46
1:B:171:MET:SD	1:B:241:GLN:HG3	2.55	0.46
1:B:380:TYR:HB2	1:B:407:TRP:HB3	1.97	0.46
1:B:471:ARG:HD3	1:B:527:PRO:CG	2.45	0.46
1:A:251:LEU:HD13	1:A:281:THR:OG1	2.16	0.46
1:A:546:GLY:O	1:A:550:GLY:HA3	2.16	0.45
1:B:498:THR:HB	1:B:518:PHE:CD2	2.51	0.45
1:B:362:SER:OG	1:B:497:LYS:NZ	2.46	0.45
1:A:335:GLN:HG3	1:A:336:PRO:HD2	1.98	0.45
1:A:62:ASP:O	1:A:213:ARG:HB3	2.17	0.45
1:B:428:LEU:HD13	1:B:534:THR:HG23	1.99	0.44
1:B:173:ASN:C	1:B:173:ASN:HD22	2.25	0.44
1:B:350:TYR:CE1	1:B:361:LYS:HD3	2.53	0.44
1:A:173:ASN:C	1:A:173:ASN:ND2	2.75	0.44
1:A:428:LEU:HD13	1:A:534:THR:CG2	2.48	0.44
1:B:487:GLY:HA3	1:B:518:PHE:CZ	2.53	0.43
1:B:318:ALA:CB	1:B:470:VAL:HG21	2.48	0.43
1:B:513:LYS:HD3	1:B:537:GLU:OE1	2.19	0.43
1:B:374:PHE:HB3	1:B:378:GLU:HG3	2.01	0.42
1:A:89:SER:HA	1:A:166:LYS:O	2.20	0.41
1:B:211:ARG:HG2	1:B:217:ILE:HA	2.02	0.41
1:B:173:ASN:HD22	1:B:174:LEU:N	2.18	0.41
1:A:173:ASN:HD22	1:A:174:LEU:N	2.18	0.41
1:A:281:THR:CG2	1:A:282:PRO:HA	2.51	0.41
1:B:92:THR:HB	1:B:93:GLU:CA	2.36	0.41
1:A:86:LEU:HD23	1:A:171:MET:CE	2.46	0.40
1:B:547:VAL:O	1:B:547:VAL:HG12	2.20	0.40
1:A:86:LEU:HD21	1:A:171:MET:CE	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	356/438 (81%)	321 (90%)	35 (10%)	7	12
1	B	340/438 (78%)	317 (93%)	23 (7%)	14	25
All	All	696/876 (80%)	638 (92%)	58 (8%)	10	17

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	64	ARG
1	A	74	THR
1	A	80	ASP
1	A	92	THR
1	A	167	ARG
1	A	173	ASN
1	A	182	THR
1	A	185	ASP
1	A	194	LEU
1	A	203	GLU
1	A	218	VAL
1	A	251	LEU
1	A	256	GLU
1	A	259	GLN
1	A	281	THR
1	A	293	ASP
1	A	321	LEU
1	A	332	LEU
1	A	338	LYS
1	A	362	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	373	ARG
1	A	404	LEU
1	A	424	LEU
1	A	426	LEU
1	A	431	LEU
1	A	460	ARG
1	A	472	ASN
1	A	473	LEU
1	A	512	ASN
1	A	526	ASN
1	A	539	THR
1	A	547	VAL
1	A	551	SER
1	A	561	LEU
1	B	80	ASP
1	B	93	GLU
1	B	173	ASN
1	B	194	LEU
1	B	237	LEU
1	B	241	GLN
1	B	246	LEU
1	B	256	GLU
1	B	271	ARG
1	B	298	ARG
1	B	302	VAL
1	B	306	ILE
1	B	332	LEU
1	B	349	VAL
1	B	362	SER
1	B	371	SER
1	B	390	VAL
1	B	403	LEU
1	B	417	THR
1	B	424	LEU
1	B	473	LEU
1	B	548	VAL
1	B	562	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	173	ASN
1	A	259	GLN
1	A	329	ASN
1	A	360	GLN
1	A	425	GLN
1	A	514	HIS
1	A	541	HIS
1	B	69	GLN
1	B	173	ASN
1	B	189	GLN
1	B	296	GLN
1	B	526	ASN
1	B	562	ASN

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	1.65	1 (12%)	7,12,14	1.99	2 (28%)
1	SEP	B	465	1	8,9,10	1.75	1 (12%)	7,12,14	3.00	3 (42%)

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	-	3/6/8/10	-
1	SEP	B	465	1	-	4/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	SEP	P-O1P	3.49	1.61	1.50
1	B	465	SEP	P-O1P	3.43	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	465	SEP	OG-CB-CA	6.94	114.90	108.14
1	A	465	SEP	OG-CB-CA	4.15	112.18	108.14
1	A	465	SEP	OG-P-O1P	2.35	112.78	106.44
1	B	465	SEP	O2P-P-OG	2.34	112.78	106.67
1	B	465	SEP	O3P-P-OG	2.16	112.30	106.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	465	SEP	N-CA-CB-OG
1	A	465	SEP	C-CA-CB-OG
1	B	465	SEP	N-CA-CB-OG
1	B	465	SEP	C-CA-CB-OG
1	B	465	SEP	CB-OG-P-O1P
1	A	465	SEP	CA-CB-OG-P
1	B	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	SO4	A	8	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	2	-	4,4,4	0.22	0	6,6,6	0.20	0
2	SO4	A	13	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	A	3	-	4,4,4	0.25	0	6,6,6	0.19	0
2	SO4	A	15	-	4,4,4	0.26	0	6,6,6	0.20	0
2	SO4	B	9	-	4,4,4	0.18	0	6,6,6	0.83	0
3	GOL	A	2	-	5,5,5	0.42	0	5,5,5	0.43	0
2	SO4	B	5	-	4,4,4	0.21	0	6,6,6	0.34	0
2	SO4	B	1	-	4,4,4	0.28	0	6,6,6	0.20	0
2	SO4	B	7	-	4,4,4	0.26	0	6,6,6	0.12	0
2	SO4	A	11	-	4,4,4	0.24	0	6,6,6	0.29	0
2	SO4	B	14	-	4,4,4	0.28	0	6,6,6	0.36	0
3	GOL	B	582	-	5,5,5	0.43	0	5,5,5	0.35	0
2	SO4	B	6	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	A	4	-	4,4,4	0.23	0	6,6,6	0.40	0
2	SO4	B	12	-	4,4,4	0.26	0	6,6,6	0.20	0
2	SO4	B	10	-	4,4,4	0.25	0	6,6,6	0.10	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	GOL	B	582	-	-	4/4/4/4	-
3	GOL	A	2	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	GOL	C1-C2-C3-O3
3	B	582	GOL	O1-C1-C2-O2
3	B	582	GOL	O1-C1-C2-C3
3	B	582	GOL	C1-C2-C3-O3
3	A	2	GOL	O2-C2-C3-O3
3	B	582	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	442/542 (81%)	1.04	57 (12%)	7 5	26, 46, 56, 65	1 (0%)
1	B	425/542 (78%)	1.41	86 (20%)	3 2	33, 49, 61, 71	0
All	All	867/1084 (79%)	1.22	143 (16%)	4 3	26, 48, 60, 71	1 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	ILE	6.0
1	B	218	VAL	5.7
1	B	220	SER	5.2
1	A	543	TYR	5.0
1	B	212	ASP	4.8
1	B	185	ASP	4.5
1	A	573	THR	4.4
1	B	209	VAL	4.4
1	B	219	ASP	4.4
1	B	211	ARG	4.4
1	B	490	ASP	4.3
1	B	573	THR	4.3
1	B	454	VAL	4.2
1	B	67	ARG	4.2
1	B	216	ASN	4.0
1	B	66	VAL	4.0
1	B	571	PRO	4.0
1	A	512	ASN	3.9
1	A	348	HIS	3.9
1	B	512	ASN	3.8
1	B	206	ALA	3.7
1	B	256	GLU	3.7
1	B	184	ILE	3.7
1	B	93	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	208	VAL	3.6
1	B	207	GLU	3.6
1	B	186	GLY	3.5
1	A	572	LEU	3.4
1	B	91	PRO	3.4
1	B	68	THR	3.4
1	A	328	LEU	3.3
1	B	69	GLN	3.3
1	A	469	GLU	3.3
1	B	513	LYS	3.3
1	A	411	ARG	3.3
1	B	271	ARG	3.2
1	A	342	SER	3.2
1	A	350	TYR	3.2
1	A	500	THR	3.2
1	B	536	ASP	3.1
1	A	547	VAL	3.1
1	B	92	THR	3.1
1	B	226	ASN	3.1
1	B	572	LEU	3.0
1	A	62	ASP	3.0
1	A	499	GLY	3.0
1	A	367	THR	2.9
1	A	92	THR	2.9
1	A	334	THR	2.9
1	A	332	LEU	2.9
1	A	333	ASN	2.9
1	B	567	SER	2.9
1	B	225	ARG	2.9
1	A	363	SER	2.8
1	B	502	ARG	2.8
1	B	535	ILE	2.8
1	B	417	THR	2.8
1	A	93	GLU	2.8
1	A	329	ASN	2.7
1	A	480	PRO	2.7
1	B	501	ALA	2.7
1	A	545	GLY	2.7
1	B	544	TYR	2.7
1	A	214	GLN	2.7
1	B	500	THR	2.7
1	A	293	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	222	ASP	2.7
1	B	386	LEU	2.7
1	B	230	GLN	2.7
1	B	356	ARG	2.6
1	A	352	SER	2.6
1	B	203	GLU	2.6
1	B	516	GLY	2.6
1	A	335	GLN	2.6
1	A	256	GLU	2.6
1	A	385	GLU	2.6
1	B	385	GLU	2.6
1	B	570	LYS	2.6
1	B	165	LEU	2.5
1	A	514	HIS	2.5
1	B	331	ARG	2.5
1	B	565	GLY	2.5
1	A	168[A]	HIS	2.5
1	B	547	VAL	2.5
1	A	546	GLY	2.5
1	A	61	GLY	2.5
1	A	339	ILE	2.5
1	B	233	LYS	2.4
1	B	566	ILE	2.4
1	A	501	ALA	2.4
1	B	540	ALA	2.4
1	B	545	GLY	2.4
1	B	306	ILE	2.4
1	B	318	ALA	2.4
1	A	53	THR	2.4
1	A	351	PRO	2.4
1	B	464	GLU	2.4
1	B	538	PRO	2.4
1	A	490	ASP	2.4
1	B	453	ALA	2.4
1	B	249	GLU	2.4
1	A	539	THR	2.3
1	B	423	GLY	2.3
1	B	457	GLN	2.3
1	A	337	TYR	2.3
1	A	343	PRO	2.3
1	A	541	HIS	2.3
1	B	503	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	421	GLY	2.3
1	B	438	LEU	2.3
1	B	166	LYS	2.3
1	B	419	SER	2.2
1	A	288	ARG	2.2
1	B	416	ALA	2.2
1	B	241	GLN	2.2
1	A	346	ASP	2.2
1	A	331	ARG	2.2
1	A	353	LEU	2.2
1	A	349	VAL	2.1
1	B	323	ALA	2.1
1	B	202	GLY	2.1
1	B	221	LEU	2.1
1	A	354	ASP	2.1
1	A	483	THR	2.1
1	B	71	LEU	2.1
1	A	213	ARG	2.1
1	A	184	ILE	2.1
1	B	383	TYR	2.1
1	B	261	LYS	2.1
1	B	515	VAL	2.1
1	A	426	LEU	2.1
1	A	481	GLY	2.1
1	A	484	GLY	2.1
1	B	168	HIS	2.1
1	B	290	GLY	2.0
1	A	498	THR	2.0
1	B	498	THR	2.0
1	B	514	HIS	2.0
1	B	390	VAL	2.0
1	B	424	LEU	2.0
1	B	459	LYS	2.0
1	B	367	THR	2.0
1	A	551	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	B-factors($\text{\AA}^2$)	Q<0.9
1	SEP	B	465	10/11	0.70	0.20	52,53,57,58	5
1	SEP	A	465	10/11	0.82	0.15	46,47,50,50	5

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	10	5/5	0.51	0.39	73,73,73,73	5
2	SO4	B	12	5/5	0.56	0.31	59,59,60,61	5
2	SO4	A	13	5/5	0.62	0.35	65,65,65,66	5
2	SO4	B	6	5/5	0.62	0.26	97,97,98,98	5
2	SO4	B	7	5/5	0.63	0.35	62,62,63,63	5
2	SO4	A	15	5/5	0.68	0.23	59,60,60,61	5
2	SO4	A	3	5/5	0.73	0.23	64,65,66,66	5
2	SO4	A	11	5/5	0.84	0.18	61,64,64,65	5
2	SO4	A	4	5/5	0.85	0.16	74,75,75,76	5
2	SO4	A	8	5/5	0.86	0.22	64,64,65,65	5
2	SO4	B	14	5/5	0.86	0.21	42,42,42,43	5
2	SO4	B	2	5/5	0.88	0.12	60,61,61,61	5
2	SO4	B	1	5/5	0.89	0.14	72,73,73,74	0
3	GOL	A	2	6/6	0.89	0.17	53,54,55,56	0
3	GOL	B	582	6/6	0.90	0.18	62,63,64,64	0
2	SO4	B	5	5/5	0.93	0.11	63,65,66,66	0
2	SO4	B	9	5/5	0.97	0.09	42,45,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.