



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:52 pm GMT

PDB ID : 4P1R  
Title : Crystal Structure of PDE10A with Imidazo[4,5-b]pyridines as Potent and Selective Inhibitors  
Authors : Chmait, S.  
Deposited on : 2014-02-27  
Resolution : 2.24 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

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

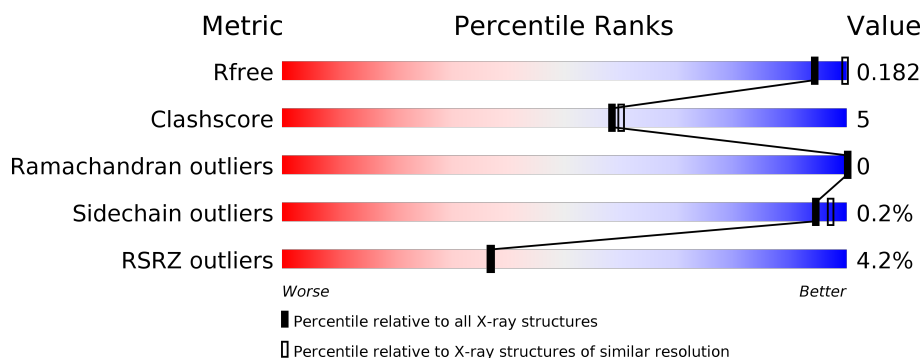
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1804 (2.26-2.22)
Clashscore	112137	1957 (2.26-2.22)
Ramachandran outliers	110173	1916 (2.26-2.22)
Sidechain outliers	110143	1917 (2.26-2.22)
RSRZ outliers	101464	1809 (2.26-2.22)

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	338	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	B	338	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </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
3	SO4	A	1003	-	-	X	X
3	SO4	A	1005	-	-	-	X
3	SO4	A	1011	-	-	-	X
3	SO4	A	1012	-	-	-	X
3	SO4	A	1013	-	-	-	X
3	SO4	A	1019	-	-	-	X
3	SO4	B	803	-	-	-	X
3	SO4	B	805	-	-	-	X
3	SO4	B	806	-	-	-	X
3	SO4	B	808	-	-	-	X
3	SO4	B	810	-	-	-	X
3	SO4	B	811	-	-	-	X
3	SO4	B	812	-	-	-	X
4	GOL	B	818	-	-	X	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6007 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.

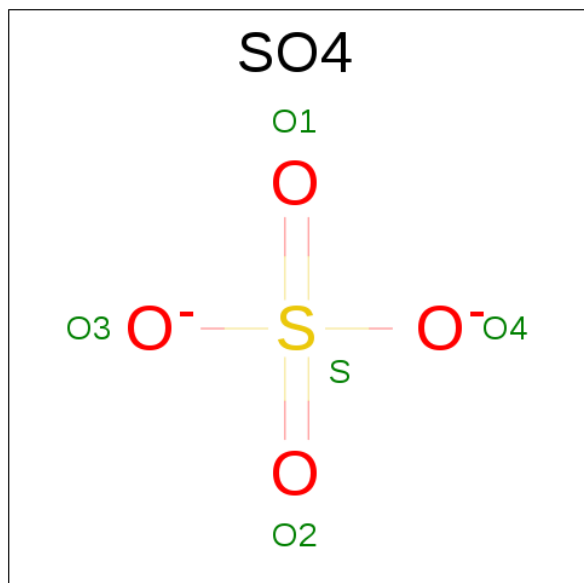
- Molecule 1 is a protein called cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2582	1650	439	470	23			
1	B	308	Total	C	N	O	S	0	1	0
			2502	1601	426	452	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

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



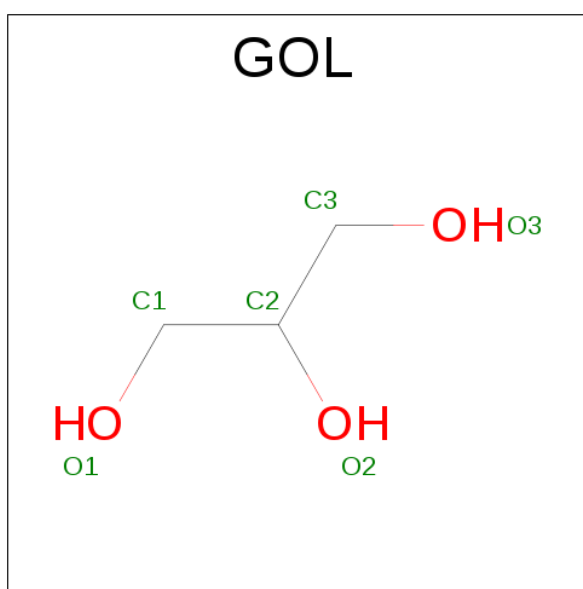
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



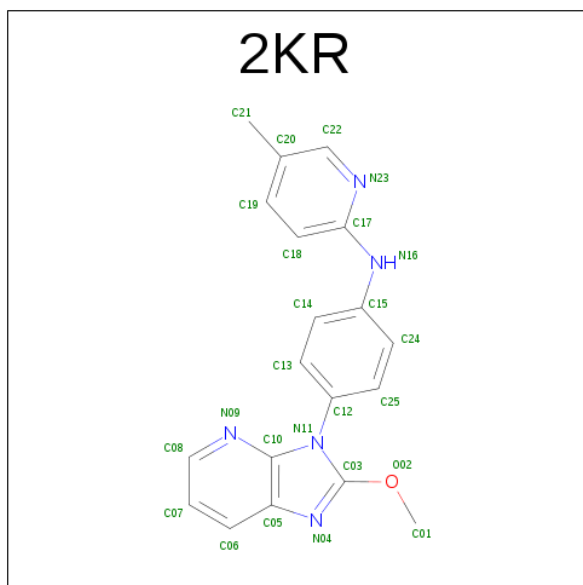
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is N-[4-(2-methoxy-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]-5-methylpyridin-2-amine (three-letter code: 2KR) (formula: C<sub>19</sub>H<sub>17</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			25	19	5	1		
5	B	1	Total	C	N	O	0	0
			25	19	5	1		

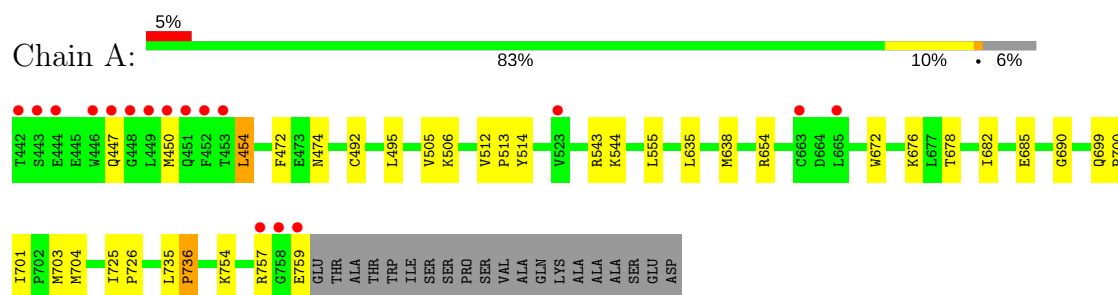
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	349	Total	O	0	0
			349	349		
6	B	342	Total	O	0	0
			342	342		

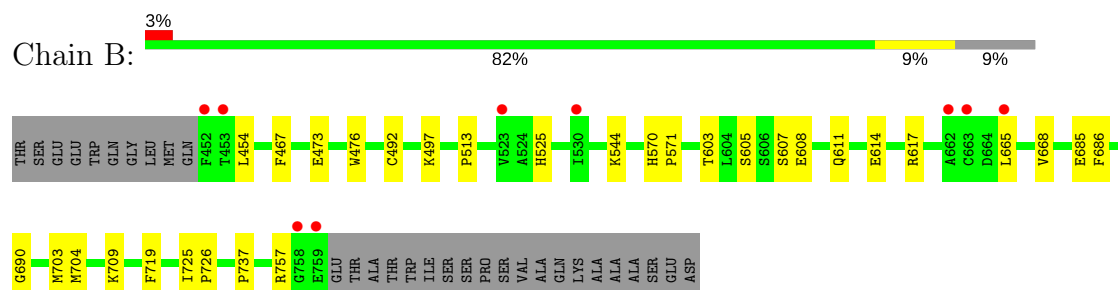
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A





## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	252.97 Å   252.97 Å   252.97 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.81 – 2.24 29.81 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.81-2.24) 99.9 (29.81-2.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.86 (at 2.24 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1589)	Depositor
R, $R_{free}$	0.153 , 0.189 0.151 , 0.182	Depositor DCC
$R_{free}$ test set	3170 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6007	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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, ZN, SO4, 2KR

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	0.64	2/2646 (0.1%)	0.60	4/3583 (0.1%)
1	B	0.48	0/2567	0.60	1/3476 (0.0%)
All	All	0.57	2/5213 (0.0%)	0.60	5/7059 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	700	PRO	N-CD	5.33	1.55	1.47
1	A	736	PRO	N-CD	5.02	1.54	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	VAL	C-N-CD	5.65	140.26	128.40
1	A	454	LEU	C-N-CD	5.64	140.24	128.40
1	A	699	GLN	C-N-CD	5.61	140.18	128.40
1	B	454	LEU	C-N-CD	5.51	139.97	128.40
1	A	735	LEU	C-N-CD	5.41	139.76	128.40

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	2582	0	2545	27	0
1	B	2502	0	2477	25	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	60	0	0	2	0
3	B	70	0	0	1	0
4	A	30	0	40	6	0
4	B	18	0	24	7	0
5	A	25	0	17	1	0
5	B	25	0	17	2	0
6	A	349	0	0	5	0
6	B	342	0	0	5	0
All	All	6007	0	5120	57	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 (57) 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:B:703:MET:HB2	4:B:819:GOL:H12	1.26	1.09
1:A:654:ARG:HE	4:A:1014:GOL:H31	1.21	1.04
1:A:736:PRO:HG2	4:B:818:GOL:H2	1.53	0.89
1:B:703:MET:HB2	4:B:819:GOL:C1	2.08	0.84
1:A:654:ARG:HE	4:A:1014:GOL:C3	1.90	0.83
1:A:736:PRO:CG	4:B:818:GOL:H2	2.12	0.80
1:B:703:MET:HG2	1:B:704:MET:CE	2.13	0.79
1:A:654:ARG:NE	4:A:1014:GOL:H31	1.99	0.78
1:A:513:PRO:HD2	1:A:685:GLU:HG3	1.65	0.78
1:A:447:GLN:NE2	6:A:1376:HOH:O	2.17	0.77
1:B:703:MET:HG2	1:B:704:MET:HE3	1.67	0.76
1:B:757:ARG:NH1	6:B:1207:HOH:O	2.22	0.72
1:A:474:ASN:ND2	3:A:1003:SO4:O3	2.24	0.71
1:A:757:ARG:NH2	1:A:759:GLU:OE1	2.24	0.69
1:B:603:THR:OG1	6:B:1188:HOH:O	2.14	0.65
4:A:1018:GOL:H32	6:A:1437:HOH:O	1.96	0.64
1:B:703:MET:CG	1:B:704:MET:HE3	2.28	0.63
1:A:450:MET:HE1	1:A:495:LEU:HD22	1.81	0.62
4:A:1018:GOL:H31	5:A:1020:2KR:H10	1.82	0.61
1:A:513:PRO:HD2	1:A:685:GLU:CG	2.32	0.58
1:A:635:LEU:HA	1:A:638:MET:HE3	1.85	0.58
1:A:757:ARG:HH21	1:A:759:GLU:CD	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1018:GOL:C3	6:A:1437:HOH:O	2.50	0.57
1:A:678:THR:O	1:A:682:ILE:HD12	2.04	0.57
4:B:818:GOL:H12	6:B:1153:HOH:O	2.04	0.57
1:B:709:LYS:NZ	6:B:1146:HOH:O	2.37	0.57
1:B:737:PRO:HB3	4:B:818:GOL:H11	1.87	0.56
4:B:819:GOL:H11	5:B:820:2KR:H10	1.88	0.55
1:B:473:GLU:HG2	1:B:476:TRP:CH2	2.42	0.55
1:B:492[B]:CYS:SG	1:B:544:LYS:HG2	2.48	0.54
1:B:686:PHE:HB3	1:B:704:MET:HE2	1.90	0.54
1:B:614:GLU:OE2	1:B:617:ARG:NH2	2.27	0.53
1:B:719:PHE:CD1	5:B:820:2KR:H17	2.44	0.53
1:B:605:SER:OG	1:B:608:GLU:HG3	2.09	0.52
1:B:467:PHE:HB3	1:B:525:HIS:CE1	2.44	0.52
1:B:607:SER:O	1:B:611:GLN:HG3	2.11	0.50
1:B:513:PRO:HD2	1:B:685:GLU:HG2	1.93	0.50
1:A:736:PRO:HB2	6:B:1212:HOH:O	2.13	0.48
1:A:543:ARG:HD3	6:A:1426:HOH:O	2.13	0.47
1:B:665:LEU:O	1:B:668:VAL:HG22	2.15	0.47
1:A:757:ARG:NE	1:A:759:GLU:OE1	2.45	0.46
1:A:472:PHE:HB3	3:A:1003:SO4:O2	2.16	0.46
1:A:754:LYS:NZ	1:A:759:GLU:HG2	2.31	0.46
1:A:701:ILE:HD11	1:A:703:MET:CE	2.47	0.45
1:B:492[B]:CYS:SG	1:B:544:LYS:HE2	2.57	0.45
1:A:506:LYS:HE3	6:A:1179:HOH:O	2.15	0.44
1:B:725:ILE:HB	1:B:726:PRO:HD3	2.00	0.44
1:A:492:CYS:HB3	1:A:544:LYS:HE2	1.99	0.44
1:B:690:GLY:HA3	1:B:704:MET:O	2.17	0.44
1:B:497:LYS:NZ	3:B:807:SO4:O1	2.43	0.42
1:A:505:VAL:HG13	1:A:555:LEU:HD21	2.01	0.42
1:B:686:PHE:CD2	1:B:704:MET:HE1	2.55	0.42
1:A:690:GLY:HA3	1:A:704:MET:O	2.20	0.41
1:A:672:TRP:CH2	1:A:676:LYS:HD3	2.55	0.41
1:B:570:HIS:CG	1:B:571:PRO:HD2	2.57	0.40
1:A:725:ILE:HB	1:A:726:PRO:HD3	2.04	0.40
1:A:514:TYR:CD1	1:A:682:ILE:HG13	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	316/338 (94%)	312 (99%)	4 (1%)	0	100	100
1	B	307/338 (91%)	301 (98%)	6 (2%)	0	100	100
All	All	623/676 (92%)	613 (98%)	10 (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	287/302 (95%)	286 (100%)	1 (0%)	94	96
1	B	279/302 (92%)	279 (100%)	0	100	100
All	All	566/604 (94%)	565 (100%)	1 (0%)	94	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	454	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	714	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 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	SO4	A	1003	-	4,4,4	0.19	0	6,6,6	0.24	0
3	SO4	A	1004	-	4,4,4	0.13	0	6,6,6	0.27	0
3	SO4	A	1005	-	4,4,4	0.12	0	6,6,6	0.28	0
3	SO4	A	1006	-	4,4,4	0.16	0	6,6,6	0.22	0
3	SO4	A	1007	-	4,4,4	0.18	0	6,6,6	0.10	0
3	SO4	A	1008	-	4,4,4	0.17	0	6,6,6	0.16	0
3	SO4	A	1009	-	4,4,4	0.19	0	6,6,6	0.09	0
3	SO4	A	1010	-	4,4,4	0.20	0	6,6,6	0.11	0
3	SO4	A	1011	-	4,4,4	0.17	0	6,6,6	0.19	0
3	SO4	A	1012	-	4,4,4	0.15	0	6,6,6	0.32	0
3	SO4	A	1013	-	4,4,4	0.15	0	6,6,6	0.41	0
4	GOL	A	1014	-	5,5,5	0.13	0	5,5,5	0.40	0
4	GOL	A	1015	-	5,5,5	0.31	0	5,5,5	0.34	0
4	GOL	A	1016	-	5,5,5	0.36	0	5,5,5	0.44	0
4	GOL	A	1017	-	5,5,5	0.27	0	5,5,5	0.65	0
4	GOL	A	1018	-	5,5,5	0.14	0	5,5,5	0.45	0
3	SO4	A	1019	-	4,4,4	0.17	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	2KR	A	1020	-	26,28,28	2.31	5 (19%)	26,39,39	1.93	5 (19%)
3	SO4	B	803	-	4,4,4	0.21	0	6,6,6	0.27	0
3	SO4	B	804	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	B	805	-	4,4,4	0.21	0	6,6,6	0.13	0
3	SO4	B	806	-	4,4,4	0.21	0	6,6,6	0.09	0
3	SO4	B	807	-	4,4,4	0.14	0	6,6,6	0.26	0
3	SO4	B	808	-	4,4,4	0.20	0	6,6,6	0.07	0
3	SO4	B	809	-	4,4,4	0.16	0	6,6,6	0.17	0
3	SO4	B	810	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	B	811	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	B	812	-	4,4,4	0.21	0	6,6,6	0.13	0
3	SO4	B	813	-	4,4,4	0.19	0	6,6,6	0.13	0
3	SO4	B	814	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	815	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	816	-	4,4,4	0.21	0	6,6,6	0.18	0
4	GOL	B	817	-	5,5,5	0.34	0	5,5,5	0.44	0
4	GOL	B	818	-	5,5,5	0.14	0	5,5,5	0.28	0
4	GOL	B	819	-	5,5,5	0.11	0	5,5,5	0.35	0
5	2KR	B	820	-	26,28,28	2.40	6 (23%)	26,39,39	1.64	5 (19%)

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	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1006	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1007	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1008	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1009	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1010	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1011	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1012	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1013	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1014	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1015	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1016	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1017	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1018	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1019	-	-	0/0/0/0	0/0/0/0
5	2KR	A	1020	-	-	0/8/10/10	0/4/4/4
3	SO4	B	803	-	-	0/0/0/0	0/0/0/0
3	SO4	B	804	-	-	0/0/0/0	0/0/0/0
3	SO4	B	805	-	-	0/0/0/0	0/0/0/0
3	SO4	B	806	-	-	0/0/0/0	0/0/0/0
3	SO4	B	807	-	-	0/0/0/0	0/0/0/0
3	SO4	B	808	-	-	0/0/0/0	0/0/0/0
3	SO4	B	809	-	-	0/0/0/0	0/0/0/0
3	SO4	B	810	-	-	0/0/0/0	0/0/0/0
3	SO4	B	811	-	-	0/0/0/0	0/0/0/0
3	SO4	B	812	-	-	0/0/0/0	0/0/0/0
3	SO4	B	813	-	-	0/0/0/0	0/0/0/0
3	SO4	B	814	-	-	0/0/0/0	0/0/0/0
3	SO4	B	815	-	-	0/0/0/0	0/0/0/0
3	SO4	B	816	-	-	0/0/0/0	0/0/0/0
4	GOL	B	817	-	-	0/4/4/4	0/0/0/0
4	GOL	B	818	-	-	0/4/4/4	0/0/0/0
4	GOL	B	819	-	-	0/4/4/4	0/0/0/0
5	2KR	B	820	-	-	0/8/10/10	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1020	2KR	C12-N11	-6.82	1.36	1.46
5	B	820	2KR	C12-N11	-6.59	1.36	1.46
5	B	820	2KR	C10-N09	2.13	1.38	1.35
5	B	820	2KR	C15-N16	2.15	1.45	1.40
5	A	1020	2KR	C15-N16	2.23	1.45	1.40
5	A	1020	2KR	C07-C06	2.24	1.41	1.36
5	B	820	2KR	C07-C06	2.49	1.42	1.36
5	B	820	2KR	C17-N16	3.31	1.44	1.38
5	A	1020	2KR	C17-N16	3.46	1.44	1.38
5	A	1020	2KR	O02-C03	6.81	1.43	1.33
5	B	820	2KR	O02-C03	7.74	1.45	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1020	2KR	C01-O02-C03	-5.51	112.35	117.44
5	A	1020	2KR	C20-C22-N23	-3.78	120.37	124.80
5	B	820	2KR	C20-C22-N23	-3.77	120.37	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	820	2KR	C18-C19-C20	-2.94	117.50	121.39
5	A	1020	2KR	C18-C19-C20	-2.90	117.56	121.39
5	B	820	2KR	C01-O02-C03	-2.05	115.54	117.44
5	A	1020	2KR	C22-N23-C17	2.77	120.79	117.91
5	B	820	2KR	C22-N23-C17	2.83	120.85	117.91
5	B	820	2KR	C08-N09-C10	2.98	120.86	116.80
5	A	1020	2KR	C08-N09-C10	3.29	121.27	116.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	SO4	2	0
4	A	1014	GOL	3	0
4	A	1018	GOL	3	0
5	A	1020	2KR	1	0
3	B	807	SO4	1	0
4	B	818	GOL	4	0
4	B	819	GOL	3	0
5	B	820	2KR	2	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	318/338 (94%)	-0.22	17 (5%) 27 27	23, 31, 57, 87	0
1	B	308/338 (91%)	-0.27	9 (2%) 52 53	22, 32, 47, 75	0
All	All	626/676 (92%)	-0.25	26 (4%) 37 37	22, 31, 50, 87	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	TRP	5.8
1	A	452	PHE	5.4
1	A	450	MET	5.0
1	A	759	GLU	4.8
1	A	449	LEU	4.7
1	A	451	GLN	4.3
1	B	759	GLU	4.1
1	B	758	GLY	4.0
1	A	448	GLY	3.4
1	A	443	SER	3.4
1	B	452	PHE	3.4
1	B	453	THR	3.2
1	A	758	GLY	3.2
1	A	453	THR	3.0
1	A	447	GLN	2.8
1	A	444	GLU	2.8
1	A	665	LEU	2.7
1	A	442	THR	2.7
1	A	757	ARG	2.6
1	A	523	VAL	2.4
1	B	662	ALA	2.4
1	B	523	VAL	2.3
1	B	530	ILE	2.2
1	B	663	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	665	LEU	2.0
1	A	663	CYS	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 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(Å <sup>2</sup> )	Q<0.9
3	SO4	A	1012	5/5	0.88	0.27	25.67	66,68,79,90	0
3	SO4	B	810	5/5	0.90	0.34	20.03	69,72,74,75	0
3	SO4	B	806	5/5	0.88	0.31	19.24	77,77,79,85	0
4	GOL	B	818	6/6	0.88	0.36	11.06	43,50,55,59	0
3	SO4	A	1013	5/5	0.91	0.33	8.28	72,74,83,85	0
3	SO4	A	1005	5/5	0.89	0.18	7.44	39,40,46,52	5
3	SO4	B	808	5/5	0.82	0.33	6.98	69,71,79,83	0
3	SO4	A	1019	5/5	0.96	0.32	6.36	82,82,85,93	0
3	SO4	B	805	5/5	0.87	0.31	6.23	73,75,76,88	0
3	SO4	A	1003	5/5	0.96	0.36	5.87	50,51,53,62	0
3	SO4	B	812	5/5	0.83	0.27	5.83	70,71,77,88	0
3	SO4	B	811	5/5	0.91	0.33	5.61	77,77,84,89	0
3	SO4	B	803	5/5	0.97	0.23	5.13	44,47,49,55	0
3	SO4	A	1011	5/5	0.95	0.28	2.17	68,69,76,87	0
3	SO4	A	1006	5/5	0.92	0.12	0.33	58,60,64,74	0
3	SO4	A	1004	5/5	0.99	0.09	-0.26	41,42,44,45	0
4	GOL	A	1015	6/6	0.93	0.10	-0.37	37,40,45,51	0
5	2KR	A	1020	25/25	0.95	0.11	-0.40	28,31,34,37	0
3	SO4	B	807	5/5	0.99	0.10	-0.42	44,45,49,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	2KR	B	820	25/25	0.96	0.11	-0.57	27,33,37,39	0
4	GOL	B	817	6/6	0.96	0.09	-0.95	39,42,46,47	0
2	ZN	B	801	1/1	1.00	0.07	-2.01	33,33,33,33	0
2	ZN	A	1002	1/1	1.00	0.05	-2.05	37,37,37,37	0
2	ZN	A	1001	1/1	1.00	0.06	-2.07	32,32,32,32	0
2	ZN	B	802	1/1	1.00	0.05	-3.24	37,37,37,37	0
3	SO4	B	815	5/5	0.98	0.15	-	37,37,38,38	5
4	GOL	B	819	6/6	0.82	0.47	-	69,72,77,82	0
3	SO4	B	813	5/5	0.85	0.51	-	72,74,88,100	0
4	GOL	A	1018	6/6	0.87	0.43	-	42,58,60,64	0
3	SO4	B	809	5/5	0.96	0.31	-	67,70,75,81	0
3	SO4	A	1009	5/5	0.96	0.27	-	81,82,84,92	0
3	SO4	A	1008	5/5	0.93	0.20	-	66,68,76,87	0
3	SO4	A	1007	5/5	0.95	0.37	-	60,70,72,80	0
3	SO4	A	1010	5/5	0.93	0.37	-	67,68,81,82	0
4	GOL	A	1014	6/6	0.84	0.29	-	51,61,65,74	0
3	SO4	B	814	5/5	0.87	0.49	-	68,78,83,99	0
4	GOL	A	1016	6/6	0.94	0.14	-	47,54,59,62	0
3	SO4	B	804	5/5	0.93	0.36	-	58,72,74,82	0
3	SO4	B	816	5/5	0.92	0.36	-	68,69,79,93	0
4	GOL	A	1017	6/6	0.89	0.35	-	47,48,61,64	0

## 6.5 Other polymers

There are no such residues in this entry.