



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID : 2BG6
Title : Bacillus cereus metallo-beta-lactamase (BcII) Arg (121) Cys mutant. Solved at pH5 using 20 Micromolar ZnSO4 in the buffer. 1mM DTT was used as a reducing agent. Cys221 is oxidized.
Authors : Davies, A.M.; Rasia, R.M.; Vila, A.J.; Sutton, B.J.; Fabiane, S.M.
Deposited on : 2004-12-17
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

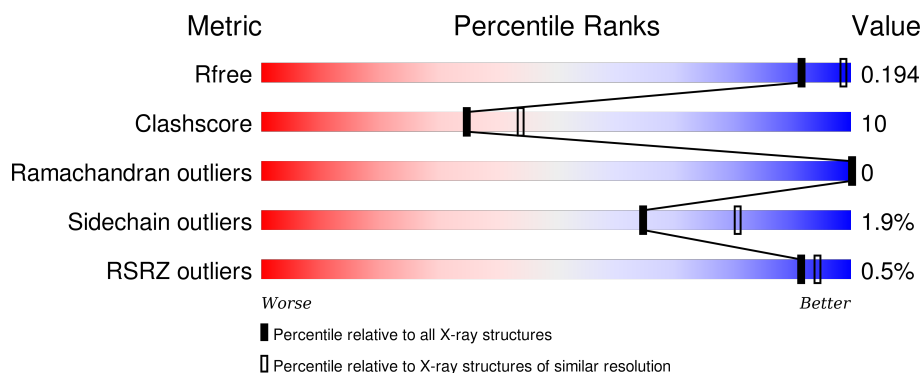
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 ≥ 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	227	
1	B	227	

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
2	GOL	A	1295	-	-	-	X
2	GOL	A	1297	-	-	-	X
2	GOL	A	1298	-	-	-	X
2	GOL	A	1300	-	-	-	X
2	GOL	B	1294	-	-	-	X
2	GOL	B	1298	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3825 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 BETA-LACTAMASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	2	0
			1686	1068	289	325	4			
1	B	218	Total	C	N	O	S	0	1	0
			1691	1071	290	325	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	CYS	ARG	ENGINEERED MUTATION	UNP P04190
B	121	CYS	ARG	ENGINEERED MUTATION	UNP P04190

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
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		
2	B	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 ZINC ION (three-letter code: ZN) (formula: Zn).

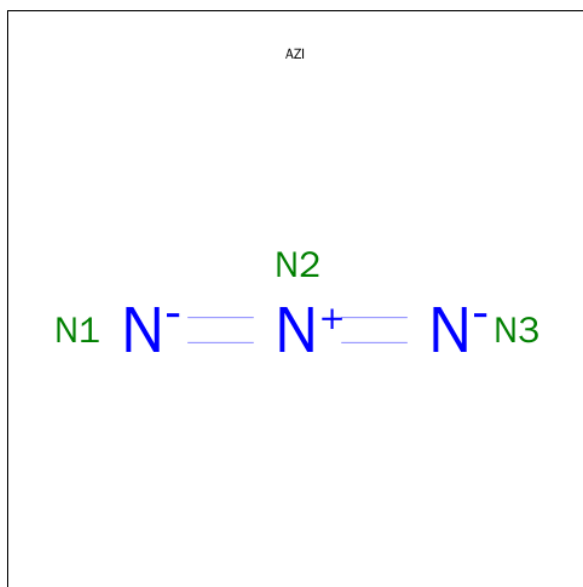
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is AZIDE ION (three-letter code: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total N 3 3	0	0
5	B	1	Total N 3 3	0	0

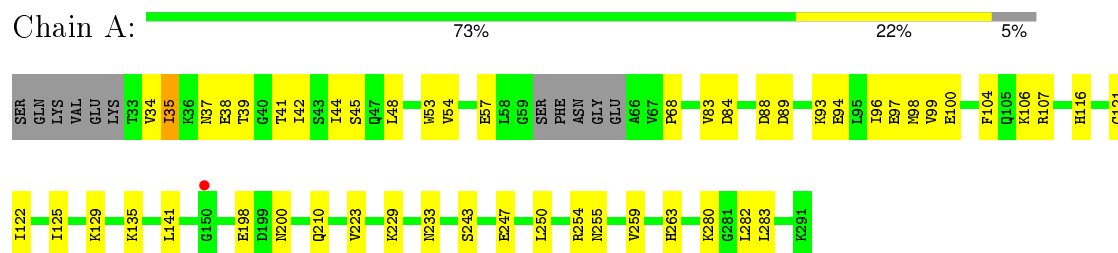
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	140	Total O 140 140	0	0
6	B	164	Total O 164 164	0	0

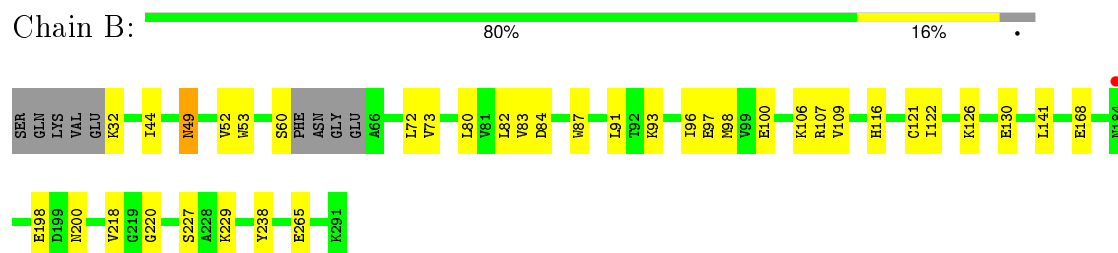
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: BETA-LACTAMASE II



• Molecule 1: BETA-LACTAMASE II



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	67.87Å 67.87Å 178.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.30 41.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (6.00-2.30) 99.6 (41.81-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.71 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.182 , 0.223 0.181 , 0.194	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.3	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 40699 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3825	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, AZI, ZN, CSD, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/1704	0.64	0/2307
1	B	0.34	0/1709	0.65	0/2313
All	All	0.34	0/3413	0.64	0/4620

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

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	1686	0	1723	38	0
1	B	1691	0	1732	34	0
2	A	60	0	37	7	0
2	B	36	0	23	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	0	0	0	0
4	B	25	0	0	2	0
5	B	6	0	0	0	0
6	A	140	0	0	1	0
6	B	164	0	0	4	0
All	All	3825	0	3515	70	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 10.

All (70) 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:229:LYS:H	2:A:1296:GOL:H12	1.39	0.87
1:A:38:GLU:CD	1:A:38:GLU:H	1.85	0.80
1:A:88:ASP:HB2	2:A:1293:GOL:C3	2.19	0.71
1:A:89:ASP:H	2:A:1293:GOL:C3	2.03	0.70
1:B:49:ASN:HD21	1:B:52:VAL:HG23	1.57	0.69
1:A:68:PRO:O	1:A:263:HIS:ND1	2.26	0.67
1:B:126:LYS:O	1:B:130:GLU:HG3	1.95	0.67
1:A:37:ASN:HB3	1:A:98:MET:HE1	1.77	0.65
1:B:44:ILE:CD1	1:B:98[A]:MET:SD	2.86	0.64
1:A:250:LEU:HD22	1:A:280:LYS:HE3	1.79	0.64
1:A:116:HIS:CE1	1:A:121:CYS:SG	2.93	0.61
1:B:32:LYS:HE2	6:B:2080:HOH:O	2.01	0.61
1:A:229:LYS:H	2:A:1296:GOL:C1	2.12	0.59
1:B:220:GLY:HA2	6:B:2141:HOH:O	2.02	0.59
1:B:265:GLU:OE2	2:B:1298:GOL:H12	2.03	0.58
1:B:107:ARG:NH1	2:B:1297:GOL:O2	2.37	0.58
1:B:49:ASN:HD21	1:B:52:VAL:CG2	2.17	0.58
1:A:83:VAL:O	1:A:84:ASP:HB2	2.05	0.57
1:B:49:ASN:HB2	2:B:1296:GOL:H11	1.86	0.57
1:A:88:ASP:HB2	2:A:1293:GOL:H12	1.89	0.55
1:A:96:ILE:O	1:A:100:GLU:HG3	2.07	0.55
1:A:135[B]:LYS:NZ	6:A:2056:HOH:O	2.40	0.54
1:B:80:LEU:HG	1:B:106:LYS:HG3	1.90	0.53
1:A:48:LEU:HB3	2:A:1298:GOL:H11	1.91	0.53
1:A:223:VAL:HG22	1:A:283:LEU:HD23	1.91	0.53
1:B:44:ILE:HG22	1:B:53:TRP:HE3	1.74	0.53
1:B:93:LYS:O	1:B:97:GLU:HG3	2.09	0.52
1:A:37:ASN:HB3	1:A:98:MET:CE	2.39	0.52
1:B:44:ILE:HG22	1:B:53:TRP:HB3	1.92	0.52
1:A:35:ILE:HD11	1:A:98:MET:SD	2.50	0.52
1:B:198:GLU:HB3	1:B:238:TYR:CE1	2.45	0.51
1:A:38:GLU:N	1:A:38:GLU:CD	2.62	0.50
1:A:210:GLN:HE21	2:A:1294:GOL:C2	2.24	0.50
1:B:116:HIS:CE1	1:B:121:CYS:SG	3.04	0.50
1:B:72:LEU:HD22	1:B:218:VAL:CG2	2.41	0.50
1:A:243:SER:O	1:A:247:GLU:HG2	2.13	0.49
1:B:168:GLU:HG2	4:B:1306:SO4:O3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:HG22	1:A:45:SER:HB3	1.95	0.48
1:A:259:VAL:HG22	1:A:282:LEU:HD12	1.95	0.48
1:B:44:ILE:HG22	1:B:53:TRP:CE3	2.48	0.48
1:B:227:SER:HB2	4:B:1302:SO4:O1	2.14	0.48
1:B:44:ILE:N	1:B:44:ILE:HD12	2.29	0.48
1:B:44:ILE:HD11	1:B:98[A]:MET:SD	2.53	0.47
1:B:96:ILE:O	1:B:100:GLU:HG3	2.14	0.47
1:A:44:ILE:HD13	1:A:99:VAL:HG12	1.96	0.46
1:B:141:LEU:HD21	1:B:198:GLU:HG3	1.98	0.46
1:A:254:ARG:C	1:A:255:ASN:HD22	2.19	0.46
1:B:49:ASN:HA	6:B:2022:HOH:O	2.15	0.46
1:A:141:LEU:HD21	1:A:198:GLU:HG2	1.99	0.45
1:A:254:ARG:HH11	1:A:254:ARG:HG3	1.82	0.44
1:A:42:ILE:HD12	1:A:94:GLU:HG2	1.99	0.44
1:A:233:ASN:HD21	1:B:229:LYS:HD3	1.83	0.44
1:A:233:ASN:ND2	1:B:229:LYS:HD3	2.33	0.43
1:A:122:ILE:O	1:A:122:ILE:HG12	2.18	0.43
1:A:93:LYS:O	1:A:97:GLU:HG3	2.18	0.43
1:A:48:LEU:HG	1:A:54:VAL:HG23	2.01	0.43
1:B:80:LEU:HB2	1:B:109:VAL:HA	2.01	0.43
1:B:32:LYS:NZ	6:B:2001:HOH:O	2.51	0.42
1:A:44:ILE:HG22	1:A:53:TRP:CE3	2.54	0.42
1:B:87:TRP:HB2	1:B:91:LEU:HD12	2.01	0.42
1:A:104:PHE:O	1:A:106:LYS:HG3	2.20	0.42
1:A:48:LEU:HA	1:A:48:LEU:HD23	1.92	0.41
1:B:32:LYS:HD3	1:B:32:LYS:HA	1.92	0.41
1:B:83:VAL:O	1:B:84:ASP:HB2	2.20	0.41
1:B:122:ILE:HG12	1:B:122:ILE:O	2.20	0.41
1:B:72:LEU:HD22	1:B:218:VAL:HG21	2.02	0.41
1:A:41:THR:O	1:A:57:GLU:HA	2.21	0.41
1:B:73:VAL:HG22	1:B:82:LEU:HD22	2.03	0.41
1:A:254:ARG:HD3	1:A:254:ARG:HA	1.89	0.40
1:A:125:ILE:O	1:A:129:LYS:HG3	2.21	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	213/227 (94%)	203 (95%)	10 (5%)	0	100	100
1	B	214/227 (94%)	207 (97%)	7 (3%)	0	100	100
All	All	427/454 (94%)	410 (96%)	17 (4%)	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	187/195 (96%)	183 (98%)	4 (2%)	61	78
1	B	188/195 (96%)	185 (98%)	3 (2%)	70	84
All	All	375/390 (96%)	368 (98%)	7 (2%)	65	81

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	39	THR
1	A	107	ARG
1	A	200	ASN
1	B	49	ASN
1	B	60	SER
1	B	200	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
1	B	49	ASN
1	B	215	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	CSD	A	221	1	3,7,8	0.83	0	3,8,10	1.21	0
1	CSD	B	221	1	3,7,8	0.76	0	3,8,10	1.28	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
1	CSD	A	221	1	-	1/2/6/8	0/0/0/0
1	CSD	B	221	1	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	221	CSD	CA-CB-SG-OD1
1	B	221	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 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	$\# Z > 2$
2	GOL	A	1293	-	5,5,5	4.87	5 (100%)	5,5,5	0.55	0
2	GOL	A	1294	-	5,5,5	4.70	5 (100%)	5,5,5	0.38	0
2	GOL	A	1295	-	5,5,5	4.16	4 (80%)	5,5,5	0.34	0
2	GOL	A	1296	-	5,5,5	4.36	4 (80%)	5,5,5	0.33	0
2	GOL	A	1297	-	5,5,5	4.19	4 (80%)	5,5,5	0.88	0
2	GOL	A	1298	-	5,5,5	4.53	4 (80%)	5,5,5	0.34	0
2	GOL	A	1299	-	5,5,5	4.07	5 (100%)	5,5,5	0.36	0
2	GOL	A	1300	-	5,5,5	4.87	5 (100%)	5,5,5	0.57	0
4	SO4	A	1302	-	4,4,4	0.06	0	6,6,6	0.11	0
4	SO4	A	1303	-	4,4,4	0.17	0	6,6,6	0.09	0
4	SO4	A	1304	-	4,4,4	0.23	0	6,6,6	0.07	0
2	GOL	A	1313	-	5,5,5	4.58	4 (80%)	5,5,5	0.79	0
2	GOL	A	1318	-	5,5,5	4.30	4 (80%)	5,5,5	0.64	0
2	GOL	B	1293	-	5,5,5	4.34	5 (100%)	5,5,5	0.43	0
2	GOL	B	1294	-	5,5,5	4.37	4 (80%)	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	1295	-	5,5,5	4.83	4 (80%)	5,5,5	0.52	0
2	GOL	B	1296	-	5,5,5	4.94	4 (80%)	5,5,5	0.62	0
2	GOL	B	1297	-	5,5,5	4.52	4 (80%)	5,5,5	0.59	0
2	GOL	B	1298	-	5,5,5	4.80	4 (80%)	5,5,5	0.67	0
5	AZI	B	1299	-	0,2,2	0.00	-	0,1,1	0.00	-
5	AZI	B	1300	-	0,2,2	0.00	-	0,1,1	0.00	-
4	SO4	B	1302	-	4,4,4	0.19	0	6,6,6	0.17	0
4	SO4	B	1303	-	4,4,4	0.17	0	6,6,6	0.09	0
4	SO4	B	1304	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	B	1305	-	4,4,4	0.22	0	6,6,6	0.08	0
4	SO4	B	1306	-	4,4,4	0.26	0	6,6,6	0.06	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	A	1293	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1294	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1295	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1296	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1297	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1298	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1299	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1300	-	-	0/4/4/4	0/0/0/0
4	SO4	A	1302	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1303	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1304	-	-	0/0/0/0	0/0/0/0
2	GOL	A	1313	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1318	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1293	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1294	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1295	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1296	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1297	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1298	-	-	0/4/4/4	0/0/0/0
5	AZI	B	1299	-	-	0/0/0/0	0/0/0/0
5	AZI	B	1300	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1302	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1303	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1304	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	B	1305	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1306	-	-	0/0/0/0	0/0/0/0

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1293	GOL	C3-C2	-8.85	1.18	1.52
2	B	1296	GOL	C3-C2	-8.71	1.19	1.52
2	A	1300	GOL	C3-C2	-8.31	1.20	1.52
2	B	1295	GOL	C3-C2	-8.15	1.21	1.52
2	B	1298	GOL	C3-C2	-8.12	1.21	1.52
2	A	1298	GOL	C3-C2	-8.10	1.21	1.52
2	B	1297	GOL	C3-C2	-8.06	1.21	1.52
2	A	1296	GOL	C3-C2	-7.69	1.22	1.52
2	A	1294	GOL	C3-C2	-7.67	1.23	1.52
2	B	1294	GOL	C3-C2	-7.63	1.23	1.52
2	A	1313	GOL	C3-C2	-7.62	1.23	1.52
2	A	1318	GOL	C3-C2	-7.60	1.23	1.52
2	A	1295	GOL	C3-C2	-7.38	1.24	1.52
2	B	1293	GOL	C3-C2	-7.17	1.24	1.52
2	A	1297	GOL	C3-C2	-7.10	1.25	1.52
2	A	1299	GOL	C3-C2	-6.83	1.26	1.52
2	B	1298	GOL	C1-C2	-4.52	1.35	1.52
2	A	1313	GOL	C1-C2	-4.36	1.35	1.52
2	B	1295	GOL	C1-C2	-4.16	1.36	1.52
2	B	1295	GOL	O1-C1	-4.08	1.24	1.42
2	B	1296	GOL	C1-C2	-4.00	1.37	1.52
2	A	1300	GOL	C1-C2	-3.96	1.37	1.52
2	B	1298	GOL	O1-C1	-3.95	1.25	1.42
2	B	1296	GOL	O1-C1	-3.84	1.25	1.42
2	A	1313	GOL	O1-C1	-3.83	1.25	1.42
2	A	1300	GOL	O1-C1	-3.83	1.25	1.42
2	A	1297	GOL	O1-C1	-3.78	1.26	1.42
2	B	1294	GOL	O1-C1	-3.72	1.26	1.42
2	A	1294	GOL	O1-C1	-3.72	1.26	1.42
2	A	1293	GOL	O1-C1	-3.61	1.26	1.42
2	B	1293	GOL	O1-C1	-3.58	1.26	1.42
2	A	1294	GOL	O2-C2	-3.50	1.33	1.43
2	A	1297	GOL	C1-C2	-3.49	1.39	1.52
2	A	1295	GOL	O1-C1	-3.47	1.27	1.42
2	A	1296	GOL	O1-C1	-3.47	1.27	1.42
2	B	1294	GOL	C1-C2	-3.40	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1298	GOL	C1-C2	-3.40	1.39	1.52
2	A	1318	GOL	C1-C2	-3.39	1.39	1.52
2	B	1297	GOL	O1-C1	-3.37	1.27	1.42
2	A	1298	GOL	O1-C1	-3.36	1.27	1.42
2	A	1299	GOL	O1-C1	-3.30	1.28	1.42
2	A	1318	GOL	O1-C1	-3.28	1.28	1.42
2	B	1297	GOL	C1-C2	-3.26	1.39	1.52
2	A	1294	GOL	C1-C2	-3.18	1.40	1.52
2	A	1293	GOL	C1-C2	-3.08	1.40	1.52
2	B	1293	GOL	C1-C2	-3.02	1.40	1.52
2	A	1296	GOL	C1-C2	-2.93	1.41	1.52
2	B	1293	GOL	O2-C2	-2.73	1.35	1.43
2	A	1295	GOL	C1-C2	-2.71	1.42	1.52
2	A	1293	GOL	O2-C2	-2.53	1.35	1.43
2	A	1299	GOL	O2-C2	-2.29	1.36	1.43
2	A	1300	GOL	O2-C2	-2.27	1.36	1.43
2	A	1299	GOL	C1-C2	-2.21	1.43	1.52
2	A	1295	GOL	O3-C3	3.19	1.56	1.42
2	B	1294	GOL	O3-C3	3.22	1.56	1.42
2	A	1297	GOL	O3-C3	3.22	1.56	1.42
2	B	1298	GOL	O3-C3	3.24	1.56	1.42
2	A	1313	GOL	O3-C3	3.28	1.56	1.42
2	A	1298	GOL	O3-C3	3.31	1.56	1.42
2	A	1293	GOL	O3-C3	3.34	1.56	1.42
2	A	1318	GOL	O3-C3	3.34	1.56	1.42
2	B	1297	GOL	O3-C3	3.49	1.57	1.42
2	A	1296	GOL	O3-C3	3.51	1.57	1.42
2	B	1296	GOL	O3-C3	3.51	1.57	1.42
2	B	1295	GOL	O3-C3	3.51	1.57	1.42
2	B	1293	GOL	O3-C3	3.64	1.58	1.42
2	A	1300	GOL	O3-C3	3.76	1.58	1.42
2	A	1299	GOL	O3-C3	3.89	1.59	1.42
2	A	1294	GOL	O3-C3	3.93	1.59	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1293	GOL	3	0
2	A	1294	GOL	1	0
2	A	1296	GOL	2	0
2	A	1298	GOL	1	0
2	B	1296	GOL	1	0
2	B	1297	GOL	1	0
2	B	1298	GOL	1	0
4	B	1302	SO4	1	0
4	B	1306	SO4	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, 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	215/227 (94%)	-0.33	1 (0%) 91 94	7, 15, 44, 54	0
1	B	217/227 (95%)	-0.37	1 (0%) 91 94	8, 17, 35, 49	0
All	All	432/454 (95%)	-0.35	2 (0%) 91 94	7, 16, 40, 54	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	GLY	3.3
1	B	184	ASN	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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	B	221	8/9	0.88	0.14	-	17,20,36,36	0
1	CSD	A	221	8/9	0.89	0.14	-	15,19,35,36	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	1300	6/6	0.61	0.37	15.08	47,50,51,51	0
2	GOL	B	1294	6/6	0.73	0.32	6.67	42,47,47,50	0
2	GOL	A	1295	6/6	0.77	0.23	5.76	46,47,47,50	0
2	GOL	A	1298	6/6	0.84	0.28	5.57	48,49,50,52	0
2	GOL	A	1297	6/6	0.66	0.27	5.08	44,45,46,47	0
2	GOL	B	1298	6/6	0.90	0.19	3.64	51,53,53,53	0
2	GOL	A	1313	6/6	0.85	0.20	1.80	44,45,46,47	0
2	GOL	A	1299	6/6	0.90	0.20	1.28	50,51,51,52	0
4	SO4	B	1302	5/5	0.98	0.15	0.94	36,38,39,39	0
4	SO4	A	1303	5/5	0.98	0.15	0.61	55,56,56,57	0
5	AZI	B	1299	3/3	0.86	0.12	0.20	37,37,37,38	0
4	SO4	A	1302	5/5	0.99	0.11	-0.22	19,20,22,24	0
2	GOL	A	1293	6/6	0.92	0.32	-	45,45,48,48	0
4	SO4	A	1304	5/5	0.91	0.17	-	98,98,98,98	0
2	GOL	B	1295	6/6	0.81	0.24	-	48,49,50,52	0
4	SO4	B	1306	5/5	0.83	0.37	-	91,91,91,91	0
5	AZI	B	1300	3/3	0.93	0.11	-	45,45,45,46	0
4	SO4	B	1305	5/5	0.92	0.19	-	89,89,90,90	0
2	GOL	A	1296	6/6	0.92	0.25	-	50,50,52,53	0
3	ZN	B	1301	1/1	0.99	0.05	-	28,28,28,28	0
2	GOL	B	1293	6/6	0.95	0.13	-	50,51,53,53	0
2	GOL	B	1296	6/6	0.89	0.13	-	53,53,54,54	0
4	SO4	B	1303	5/5	0.96	0.14	-	48,48,50,50	0
2	GOL	A	1318	6/6	0.88	0.19	-	57,57,58,60	0
2	GOL	B	1297	6/6	0.81	0.22	-	53,54,55,56	0
3	ZN	A	1301	1/1	0.99	0.03	-	29,29,29,29	0
2	GOL	A	1294	6/6	0.94	0.16	-	45,46,47,48	0
4	SO4	B	1304	5/5	0.91	0.15	-	88,89,89,89	0

6.5 Other polymers ⓘ

There are no such residues in this entry.