



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 10:05 am BST

PDB ID : 6SUJ
Title : Mutations in SsgB correlate to longitudinal cell division during sporulation of *Streptomyces coelicolor*
Authors : Xiao, X.S.; Willemse, J.
Deposited on : 2019-09-14
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

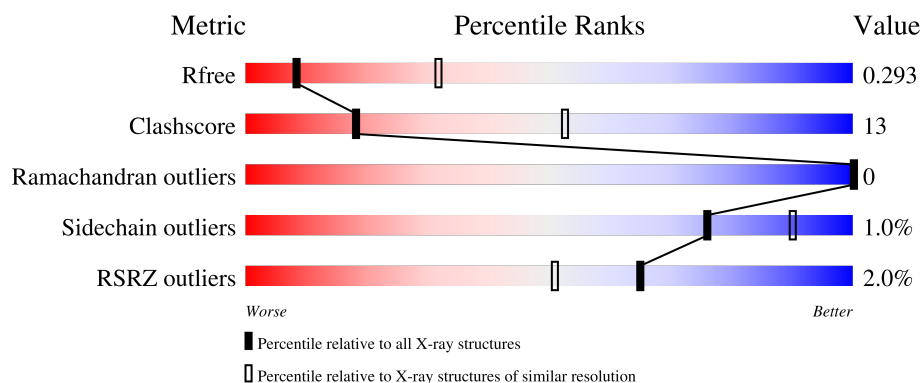
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	AAA	157	<div> <div>3%</div> <div>64% 18% 18%</div> </div>
1	BBB	157	<div> <div>3%</div> <div>66% 15% 18%</div> </div>
1	CCC	157	<div> <div>3%</div> <div>66% 15% 18%</div> </div>
1	DDD	157	<div> <div>3%</div> <div>63% 17% 20%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3967 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 Sporulation and cell division protein SsgA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	128	Total	C	N	O	S	0	0	0
			973	607	176	187	3			
1	BBB	128	Total	C	N	O	S	0	0	0
			973	607	176	187	3			
1	CCC	128	Total	C	N	O	S	0	0	0
			966	604	174	185	3			
1	DDD	126	Total	C	N	O	S	0	0	0
			954	597	175	179	3			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-19	MET	-	initiating methionine	UNP A0A3D9WLS9
AAA	-18	GLY	-	expression tag	UNP A0A3D9WLS9
AAA	-17	SER	-	expression tag	UNP A0A3D9WLS9
AAA	-16	SER	-	expression tag	UNP A0A3D9WLS9
AAA	-15	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-14	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-13	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-12	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-11	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-10	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-9	SER	-	expression tag	UNP A0A3D9WLS9
AAA	-8	SER	-	expression tag	UNP A0A3D9WLS9
AAA	-7	GLY	-	expression tag	UNP A0A3D9WLS9
AAA	-6	LEU	-	expression tag	UNP A0A3D9WLS9
AAA	-5	VAL	-	expression tag	UNP A0A3D9WLS9
AAA	-4	PRO	-	expression tag	UNP A0A3D9WLS9
AAA	-3	ARG	-	expression tag	UNP A0A3D9WLS9
AAA	-2	GLY	-	expression tag	UNP A0A3D9WLS9
AAA	-1	SER	-	expression tag	UNP A0A3D9WLS9
AAA	0	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-19	MET	-	initiating methionine	UNP A0A3D9WLS9

Continued on next page...

Continued from previous page...

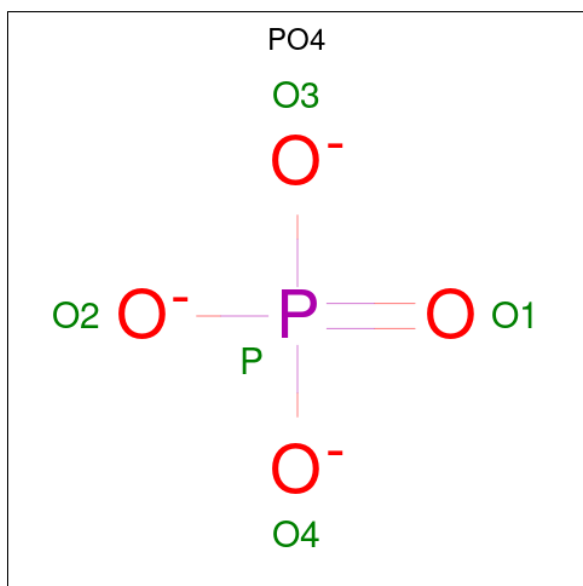
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-18	GLY	-	expression tag	UNP A0A3D9WLS9
BBB	-17	SER	-	expression tag	UNP A0A3D9WLS9
BBB	-16	SER	-	expression tag	UNP A0A3D9WLS9
BBB	-15	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-14	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-13	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-12	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-11	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-10	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-9	SER	-	expression tag	UNP A0A3D9WLS9
BBB	-8	SER	-	expression tag	UNP A0A3D9WLS9
BBB	-7	GLY	-	expression tag	UNP A0A3D9WLS9
BBB	-6	LEU	-	expression tag	UNP A0A3D9WLS9
BBB	-5	VAL	-	expression tag	UNP A0A3D9WLS9
BBB	-4	PRO	-	expression tag	UNP A0A3D9WLS9
BBB	-3	ARG	-	expression tag	UNP A0A3D9WLS9
BBB	-2	GLY	-	expression tag	UNP A0A3D9WLS9
BBB	-1	SER	-	expression tag	UNP A0A3D9WLS9
BBB	0	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-19	MET	-	initiating methionine	UNP A0A3D9WLS9
CCC	-18	GLY	-	expression tag	UNP A0A3D9WLS9
CCC	-17	SER	-	expression tag	UNP A0A3D9WLS9
CCC	-16	SER	-	expression tag	UNP A0A3D9WLS9
CCC	-15	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-14	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-13	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-12	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-11	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-10	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-9	SER	-	expression tag	UNP A0A3D9WLS9
CCC	-8	SER	-	expression tag	UNP A0A3D9WLS9
CCC	-7	GLY	-	expression tag	UNP A0A3D9WLS9
CCC	-6	LEU	-	expression tag	UNP A0A3D9WLS9
CCC	-5	VAL	-	expression tag	UNP A0A3D9WLS9
CCC	-4	PRO	-	expression tag	UNP A0A3D9WLS9
CCC	-3	ARG	-	expression tag	UNP A0A3D9WLS9
CCC	-2	GLY	-	expression tag	UNP A0A3D9WLS9
CCC	-1	SER	-	expression tag	UNP A0A3D9WLS9
CCC	0	HIS	-	expression tag	UNP A0A3D9WLS9
DDD	-19	MET	-	initiating methionine	UNP A0A3D9WLS9
DDD	-18	GLY	-	expression tag	UNP A0A3D9WLS9
DDD	-17	SER	-	expression tag	UNP A0A3D9WLS9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-16	SER	-	expression tag	UNP A0A3D9WLS9
DDD	-15	HIS	-	expression tag	UNP A0A3D9WLS9
DDD	-14	HIS	-	expression tag	UNP A0A3D9WLS9
DDD	-13	HIS	-	expression tag	UNP A0A3D9WLS9
DDD	-12	HIS	-	expression tag	UNP A0A3D9WLS9
DDD	-11	HIS	-	expression tag	UNP A0A3D9WLS9
DDD	-10	HIS	-	expression tag	UNP A0A3D9WLS9
DDD	-9	SER	-	expression tag	UNP A0A3D9WLS9
DDD	-8	SER	-	expression tag	UNP A0A3D9WLS9
DDD	-7	GLY	-	expression tag	UNP A0A3D9WLS9
DDD	-6	LEU	-	expression tag	UNP A0A3D9WLS9
DDD	-5	VAL	-	expression tag	UNP A0A3D9WLS9
DDD	-4	PRO	-	expression tag	UNP A0A3D9WLS9
DDD	-3	ARG	-	expression tag	UNP A0A3D9WLS9
DDD	-2	GLY	-	expression tag	UNP A0A3D9WLS9
DDD	-1	SER	-	expression tag	UNP A0A3D9WLS9
DDD	0	HIS	-	expression tag	UNP A0A3D9WLS9

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	DDD	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	28	Total 28	O 28	0	0
3	BBB	32	Total 32	O 32	0	0
3	CCC	16	Total 16	O 16	0	0
3	DDD	20	Total 20	O 20	0	0

V115	T119	E120	H121	R122	HIS	PHE	ASP	LEU	ASP	GLN	GLU	LEU	SER	HIS	ILE	LEU	ALA	GLU	SER
------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.93Å 93.22Å 96.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 3.20 48.12 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.17-3.20) 99.8 (48.12-3.20)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.236 , 0.293 0.239 , 0.293	Depositor DCC
R_{free} test set	550 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3967	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3005e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4

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	AAA	0.63	0/999	0.87	0/1365
1	BBB	0.63	0/999	0.84	0/1365
1	CCC	0.64	0/991	0.83	0/1356
1	DDD	0.63	0/978	0.86	0/1336
All	All	0.63	0/3967	0.85	0/5422

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	973	0	935	28	0
1	BBB	973	0	934	33	0
1	CCC	966	0	942	35	0
1	DDD	954	0	937	33	0
2	DDD	5	0	0	0	0
3	AAA	28	0	0	2	0
3	BBB	32	0	0	1	0
3	CCC	16	0	0	1	0
3	DDD	20	0	0	2	0
All	All	3967	0	3748	102	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 13.

All (102) 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:BBB:60:GLU:OE2	1:BBB:64:ARG:NH1	1.58	1.34
1:CCC:29:TYR:OH	1:CCC:115:VAL:CG1	1.88	1.21
1:CCC:29:TYR:OH	1:CCC:115:VAL:HG11	1.51	1.04
1:CCC:29:TYR:OH	1:CCC:115:VAL:HG13	1.59	1.03
1:BBB:10:HIS:CD2	1:CCC:-3:ARG:HD3	2.10	0.86
1:BBB:60:GLU:CD	1:BBB:64:ARG:NH1	2.32	0.83
1:BBB:9:LEU:HD21	1:BBB:103:ALA:CB	2.11	0.80
1:CCC:29:TYR:HH	1:CCC:115:VAL:HG11	1.50	0.73
1:BBB:9:LEU:HD21	1:BBB:103:ALA:HB1	1.71	0.73
1:DDD:121:HIS:CG	1:DDD:122:ARG:H	2.09	0.71
1:BBB:7:CYS:HB2	1:BBB:107:PHE:CD1	2.26	0.71
1:BBB:107:PHE:HA	1:CCC:1:MET:HE1	1.73	0.70
1:AAA:7:CYS:HB2	1:AAA:107:PHE:CD1	2.27	0.70
1:BBB:60:GLU:HA	1:BBB:63:HIS:CE1	2.30	0.67
1:AAA:60:GLU:OE2	1:AAA:64:ARG:NH1	2.27	0.67
1:CCC:7:CYS:HB2	1:CCC:107:PHE:CD1	2.31	0.66
1:DDD:7:CYS:HB2	1:DDD:107:PHE:CD1	2.30	0.66
1:CCC:50:GLU:O	1:DDD:0:HIS:HE1	1.79	0.65
1:CCC:120:GLU:O	1:DDD:35:TYR:CZ	2.50	0.65
1:BBB:117:PRO:HA	1:BBB:120:GLU:OE2	1.99	0.63
1:AAA:10:HIS:HB3	3:CCC:212:HOH:O	1.98	0.62
1:BBB:125:ASP:OD1	3:BBB:201:HOH:O	2.16	0.62
1:CCC:120:GLU:O	1:DDD:35:TYR:OH	2.18	0.61
1:BBB:102:ARG:NH2	1:DDD:69:GLY:HA2	2.15	0.61
1:BBB:11:LEU:CD1	1:BBB:25:ALA:CB	2.79	0.60
1:AAA:60:GLU:HA	1:AAA:63:HIS:CE1	2.37	0.60
1:AAA:62:LEU:HD23	1:AAA:84:VAL:CG2	2.33	0.59
1:BBB:62:LEU:HD23	1:BBB:84:VAL:CG2	2.32	0.59
1:AAA:11:LEU:HD23	1:AAA:99:ALA:HA	1.84	0.59
1:DDD:40:THR:HG23	1:DDD:50:GLU:HG2	1.84	0.58
1:CCC:29:TYR:CZ	1:CCC:115:VAL:CG1	2.85	0.57
1:DDD:62:LEU:HD23	1:DDD:84:VAL:CG2	2.37	0.55
1:DDD:121:HIS:CE1	1:DDD:122:ARG:HB2	2.42	0.55
1:DDD:121:HIS:ND1	1:DDD:122:ARG:N	2.55	0.55
1:BBB:10:HIS:HB3	3:DDD:310:HOH:O	2.07	0.54
1:AAA:9:LEU:HD11	1:AAA:103:ALA:CB	2.36	0.54
1:AAA:81:GLN:NE2	1:CCC:89:SER:HB3	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:84:VAL:HG21	1:BBB:104:LEU:HD23	1.89	0.54
1:BBB:11:LEU:CD1	1:BBB:25:ALA:HB2	2.38	0.54
1:BBB:60:GLU:HA	1:BBB:63:HIS:HE1	1.71	0.53
1:CCC:62:LEU:HD23	1:CCC:84:VAL:CG2	2.38	0.53
1:BBB:107:PHE:HD1	1:CCC:1:MET:HE1	1.73	0.53
1:AAA:87:ALA:HB1	1:AAA:94:GLU:OE2	2.09	0.53
1:AAA:110:ARG:NH1	3:AAA:201:HOH:O	2.38	0.52
1:BBB:11:LEU:CD1	1:BBB:25:ALA:HB3	2.39	0.52
1:DDD:84:VAL:HG21	1:DDD:104:LEU:HD23	1.92	0.52
1:BBB:81:GLN:HE22	1:BBB:102:ARG:HH12	1.58	0.51
1:DDD:119:THR:O	1:DDD:119:THR:HG22	2.09	0.51
1:BBB:11:LEU:HD13	1:BBB:25:ALA:HB2	1.92	0.51
1:AAA:84:VAL:HG21	1:AAA:104:LEU:HD23	1.91	0.51
1:AAA:1:MET:HE3	1:DDD:110:ARG:HD2	1.93	0.50
1:AAA:7:CYS:HB2	1:AAA:107:PHE:HD1	1.77	0.50
1:BBB:44:GLY:HA3	1:BBB:47:GLU:HG3	1.94	0.50
1:DDD:121:HIS:CG	1:DDD:122:ARG:N	2.77	0.49
1:BBB:0:HIS:HB2	1:CCC:8:GLU:HB2	1.95	0.49
1:AAA:1:MET:HE1	1:DDD:106:SER:C	2.34	0.48
1:CCC:35:TYR:CE1	1:DDD:121:HIS:HA	2.49	0.47
1:BBB:10:HIS:NE2	1:CCC:-3:ARG:HD3	2.30	0.47
1:AAA:88:LEU:O	1:AAA:94:GLU:HG3	2.14	0.47
1:AAA:1:MET:HE1	1:DDD:107:PHE:N	2.30	0.47
1:CCC:9:LEU:HD21	1:CCC:103:ALA:HB1	1.97	0.47
1:CCC:11:LEU:HD12	1:CCC:11:LEU:N	2.31	0.46
1:CCC:84:VAL:HG21	1:CCC:104:LEU:HD23	1.98	0.46
1:BBB:7:CYS:HB2	1:BBB:107:PHE:HD1	1.75	0.46
1:CCC:43:THR:HG21	1:DDD:-5:VAL:HB	1.98	0.46
1:BBB:107:PHE:HA	1:CCC:1:MET:CE	2.42	0.45
1:AAA:61:GLY:HA3	1:AAA:73:VAL:HG12	1.99	0.45
1:CCC:35:TYR:CZ	1:DDD:121:HIS:HA	2.51	0.45
1:DDD:42:HIS:CD2	1:DDD:48:THR:HG22	2.52	0.45
1:AAA:11:LEU:CD2	1:AAA:99:ALA:HB2	2.47	0.45
1:AAA:61:GLY:HA3	1:AAA:73:VAL:CG1	2.47	0.45
1:BBB:31:THR:HG22	1:BBB:115:VAL:CG2	2.47	0.44
1:AAA:37:VAL:HG23	1:AAA:55:ARG:CB	2.47	0.44
1:CCC:-6:LEU:CD1	3:DDD:317:HOH:O	2.65	0.44
1:AAA:11:LEU:HD12	1:AAA:25:ALA:HB2	1.99	0.44
1:BBB:60:GLU:CG	1:BBB:64:ARG:NH1	2.81	0.44
1:CCC:43:THR:HG22	1:DDD:-5:VAL:HG23	2.00	0.44
1:CCC:115:VAL:HG23	1:CCC:119:THR:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:102:ARG:NH2	1:CCC:69:GLY:HA2	2.33	0.44
1:AAA:55:ARG:HG2	3:AAA:202:HOH:O	2.16	0.43
1:DDD:11:LEU:HD12	1:DDD:11:LEU:N	2.32	0.43
1:BBB:107:PHE:CD1	1:CCC:1:MET:HE1	2.53	0.43
1:CCC:11:LEU:N	1:CCC:11:LEU:CD1	2.80	0.43
1:CCC:52:VAL:HG23	1:DDD:0:HIS:CD2	2.53	0.43
1:AAA:123:HIS:HD2	1:DDD:110:ARG:HH22	1.67	0.43
1:BBB:61:GLY:HA3	1:BBB:73:VAL:CG1	2.49	0.43
1:CCC:107:PHE:O	1:CCC:111:THR:HG23	2.19	0.43
1:DDD:31:THR:HG22	1:DDD:115:VAL:CG2	2.49	0.43
1:BBB:11:LEU:HD11	1:BBB:25:ALA:HB3	2.01	0.42
1:CCC:-4:PRO:HB3	1:DDD:90:SER:OG	2.19	0.42
1:DDD:11:LEU:N	1:DDD:11:LEU:CD1	2.82	0.42
1:AAA:1:MET:CE	1:DDD:110:ARG:HD2	2.50	0.42
1:BBB:102:ARG:CZ	1:DDD:69:GLY:HA2	2.50	0.42
1:CCC:50:GLU:O	1:DDD:0:HIS:CE1	2.66	0.42
1:AAA:9:LEU:HD11	1:AAA:103:ALA:HB1	2.02	0.41
1:CCC:90:SER:OG	1:DDD:-4:PRO:HB3	2.19	0.41
1:DDD:63:HIS:CE1	1:DDD:64:ARG:HD3	2.55	0.41
1:AAA:60:GLU:HA	1:AAA:63:HIS:HE1	1.82	0.41
1:CCC:119:THR:O	1:CCC:119:THR:HG22	2.21	0.41
1:DDD:38:HIS:ND1	1:DDD:52:VAL:HG22	2.36	0.41
1:AAA:9:LEU:CD1	1:AAA:103:ALA:HB1	2.52	0.40
1:BBB:9:LEU:HD23	1:BBB:9:LEU:HA	1.82	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	AAA	126/157 (80%)	125 (99%)	1 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	126/157 (80%)	126 (100%)	0	0	100	100
1	CCC	126/157 (80%)	123 (98%)	3 (2%)	0	100	100
1	DDD	122/157 (78%)	121 (99%)	1 (1%)	0	100	100
All	All	500/628 (80%)	495 (99%)	5 (1%)	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	AAA	104/130 (80%)	102 (98%)	2 (2%)	57	81
1	BBB	104/130 (80%)	103 (99%)	1 (1%)	76	90
1	CCC	104/130 (80%)	103 (99%)	1 (1%)	76	90
1	DDD	103/130 (79%)	103 (100%)	0	100	100
All	All	415/520 (80%)	411 (99%)	4 (1%)	76	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	16	SER
1	AAA	56	ASP
1	BBB	47	GLU
1	CCC	115	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	PO4	DDD	201	-	4,4,4	1.00	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

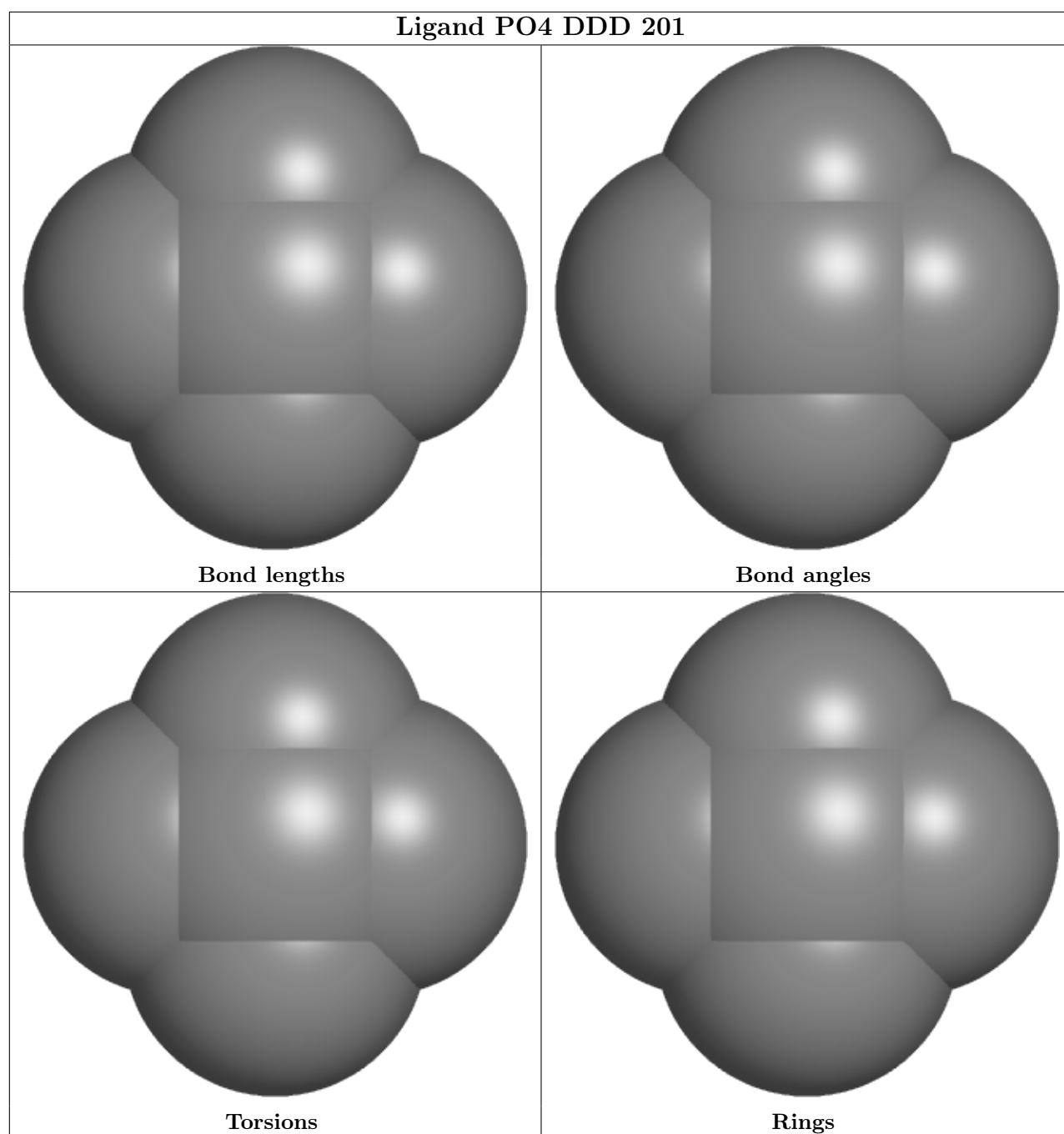
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AAA	128/157 (81%)	0.24	1 (0%) 86 78	21, 38, 73, 99	0
1	BBB	128/157 (81%)	0.21	2 (1%) 72 59	19, 36, 84, 116	0
1	CCC	128/157 (81%)	0.42	5 (3%) 39 25	25, 42, 79, 98	0
1	DDD	126/157 (80%)	0.36	2 (1%) 72 59	28, 43, 76, 105	0
All	All	510/628 (81%)	0.31	10 (1%) 65 51	19, 40, 81, 116	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	-2	GLY	5.2
1	CCC	89	SER	3.3
1	CCC	70	ASP	3.0
1	BBB	32	ALA	2.9
1	DDD	70	ASP	2.7
1	CCC	0	HIS	2.4
1	CCC	69	GLY	2.1
1	BBB	8	GLU	2.1
1	CCC	92	GLU	2.0
1	DDD	106	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

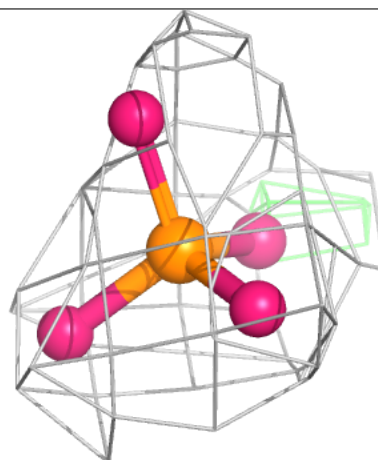
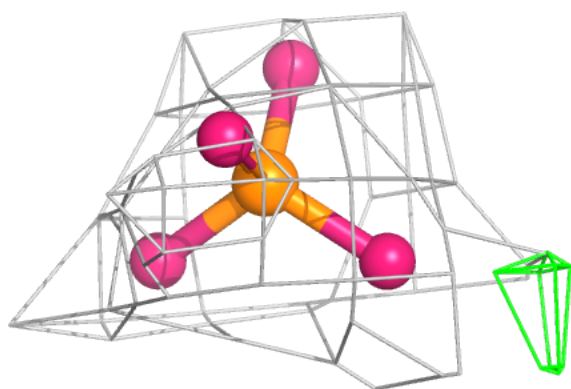
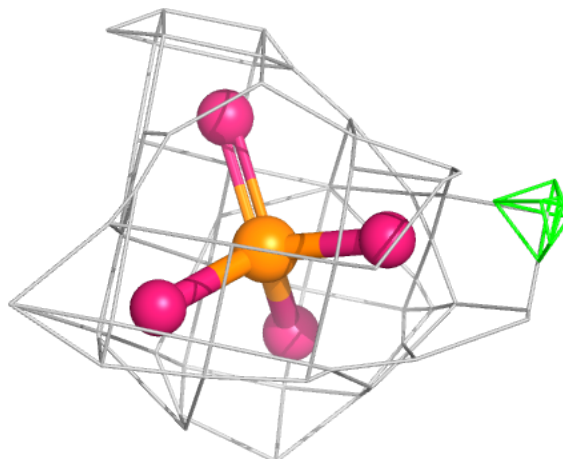
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	DDD	201	5/5	0.76	0.30	76,76,78,84	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PO4 DDD 201:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.