



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 02:21 am GMT

PDB ID : 1CS4
Title : COMPLEX OF GS-ALPHA WITH THE CATALYTIC DOMAINS OF MAMMALIAN ADENYLYL CYCLASE: COMPLEX WITH 2'-DEOXY-ADENOSINE 3'-MONOPHOSPHATE, PYROPHOSPHATE AND MG
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Deposited on : 1999-08-16
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

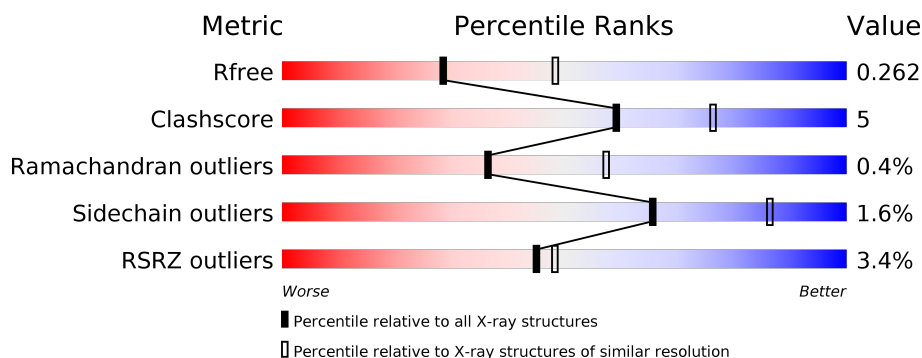
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	225	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>15%</div> <div>•</div> <div>16%</div> </div> </div>
2	B	212	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>10%</div> </div> </div>
3	C	394	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>6%</div> <div>•</div> <div>16%</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
6	MES	B	1083	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 5843 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 TYPE V ADENYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1476	929	259	271	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	476	MET	VAL	engineered	UNP P30803

- Molecule 2 is a protein called TYPE II ADENYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	0	0	0
			1479	945	243	281	10			

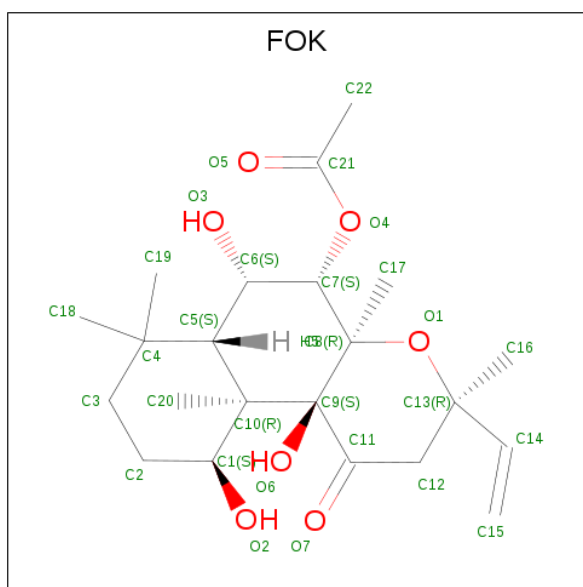
- Molecule 3 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN G(S).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	329	Total	C	N	O	S	0	0	0
			2692	1708	467	504	13			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

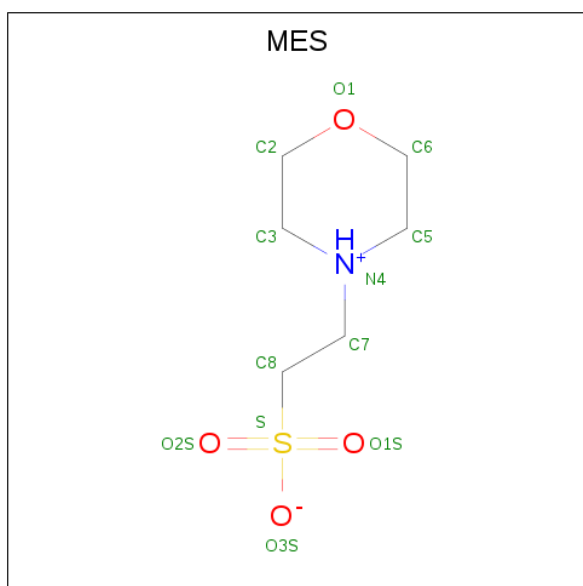
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is FORSKOLIN (three-letter code: FOK) (formula: C₂₂H₃₄O₇).



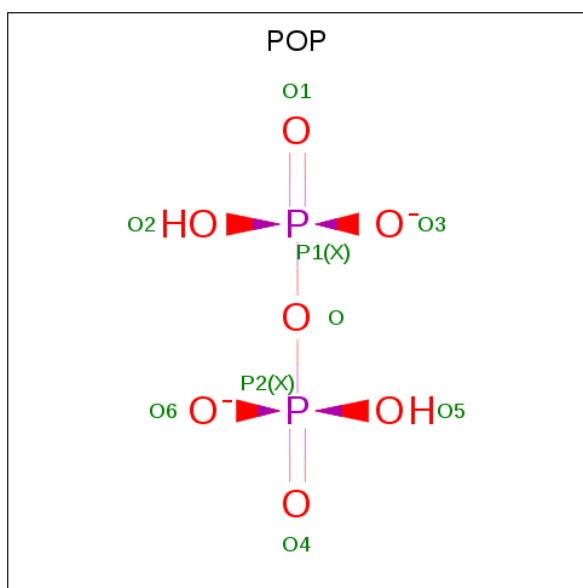
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			29	22	7		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



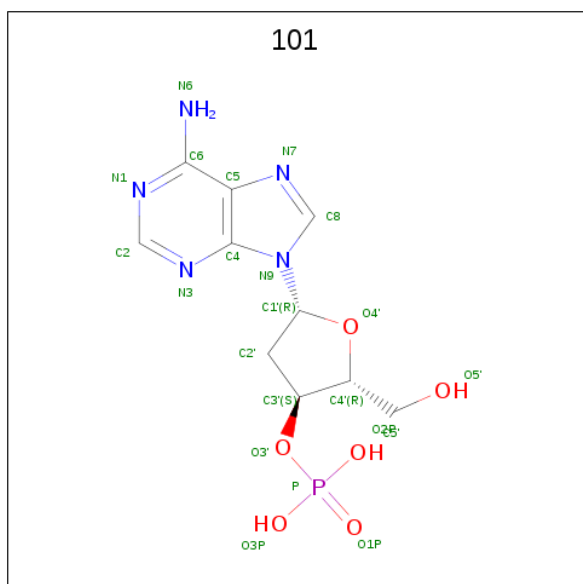
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	O	P		0	0
			9	7	2			

- Molecule 8 is 2'-DEOXY-ADENOSINE 3'-MONOPHOSPHATE (three-letter code: 101) (formula: $\text{C}_{10}\text{H}_{14}\text{N}_5\text{O}_6\text{P}$).

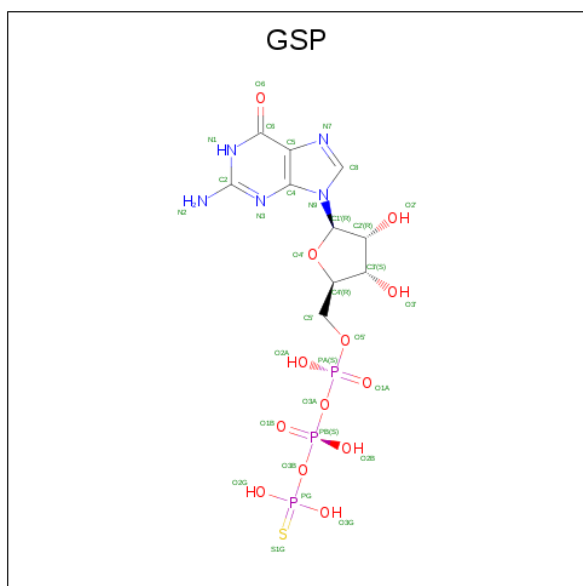


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Cl 1 1	0	0

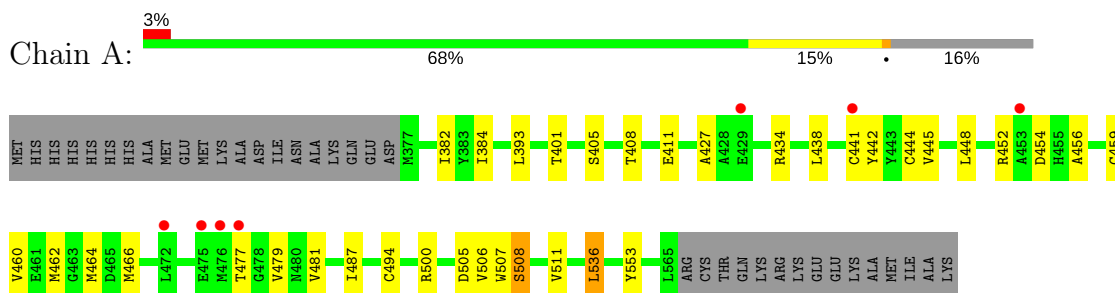
- Molecule 10 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



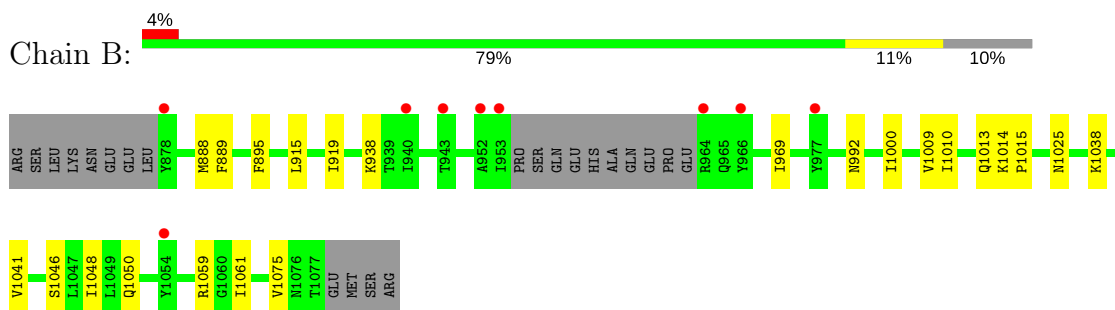
3 Residue-property plots [i](#)

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.

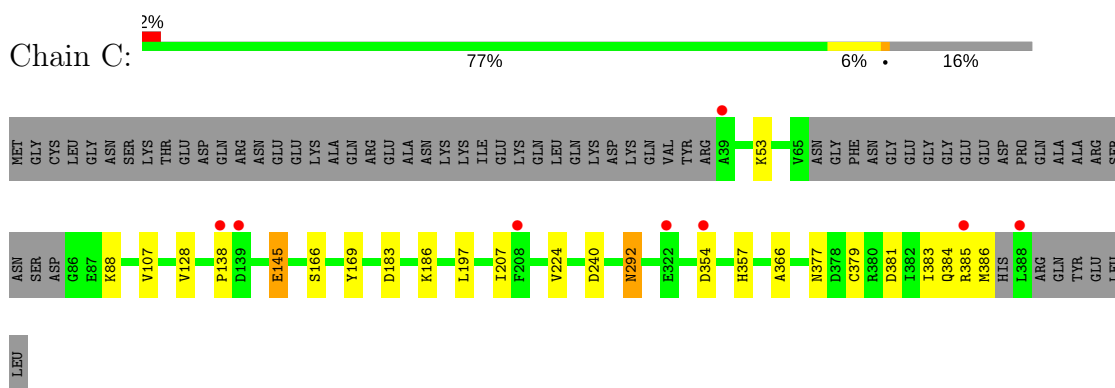
• Molecule 1: TYPE V ADENYLATE CYCLASE



• Molecule 2: TYPE II ADENYLATE CYCLASE



• Molecule 3: GUANINE NUCLEOTIDE-BINDING PROTEIN G(S)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.50Å 134.50Å 71.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 37.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.1 (15.00-2.50) 90.0 (37.95-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.264 0.218 , 0.262	Depositor DCC
R_{free} test set	7094 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	1.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5843	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: GSP, MG, CL, POP, MES, 101, FOK

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	0.35	0/1504	0.57	0/2027
2	B	0.37	0/1505	0.60	0/2032
3	C	0.38	0/2748	0.59	0/3718
All	All	0.37	0/5757	0.59	0/7777

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	A	1476	0	1450	22	0
2	B	1479	0	1479	17	0
3	C	2692	0	2643	14	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	29	0	34	7	0
6	A	12	0	13	1	0
6	B	12	0	13	3	0
7	A	9	0	0	0	0
8	B	22	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	1	0	0	0	0
10	C	32	0	12	0	0
11	A	11	0	0	0	0
11	B	31	0	0	1	0
11	C	35	0	0	0	0
All	All	5843	0	5656	58	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.

The worst 5 of 58 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)
3:C:292:ASN:HD21	3:C:366:ALA:H	1.20	0.85
5:A:1002:FOK:H201	5:A:1002:FOK:H173	1.61	0.81
3:C:381:ASP:O	3:C:385:ARG:HG2	1.90	0.70
2:B:1038:LYS:NZ	6:B:1083:MES:H31	2.07	0.69
2:B:1038:LYS:HZ2	6:B:1083:MES:H31	1.61	0.65

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	187/225 (83%)	178 (95%)	8 (4%)	1 (0%)	31	51
2	B	186/212 (88%)	180 (97%)	6 (3%)	0	100	100
3	C	325/394 (82%)	315 (97%)	8 (2%)	2 (1%)	27	46
All	All	698/831 (84%)	673 (96%)	22 (3%)	3 (0%)	36	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	SER
3	C	138	PRO
3	C	354	ASP

5.3.2 Protein sidechains [i](#)

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	158/189 (84%)	155 (98%)	3 (2%)	60	83
2	B	163/184 (89%)	161 (99%)	2 (1%)	74	90
3	C	296/351 (84%)	291 (98%)	5 (2%)	63	85
All	All	617/724 (85%)	607 (98%)	10 (2%)	65	86

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1059	ARG
3	C	145	GLU
3	C	292	ASN
2	B	992	ASN
3	C	240	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	97	ASN
3	C	149	HIS
3	C	292	ASN
3	C	93	GLN
3	C	236	GLN

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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
5	FOK	A	1002	-	28,31,31	0.78	0	32,54,54	0.85	0
6	MES	A	1003	-	12,12,12	1.07	1 (8%)	14,16,16	0.52	0
7	POP	A	1005	4	8,8,8	1.50	2 (25%)	9,13,13	0.59	0
8	101	B	1082	4	22,24,24	0.81	0	24,36,36	0.77	1 (4%)
6	MES	B	1083	-	12,12,12	1.17	1 (8%)	14,16,16	0.52	0
10	GSP	C	1000	4	26,34,34	1.06	2 (7%)	27,54,54	2.29	4 (14%)

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
5	FOK	A	1002	-	-	0/7/80/80	0/3/3/3
6	MES	A	1003	-	-	0/6/14/14	0/1/1/1
7	POP	A	1005	4	-	0/6/6/6	0/0/0/0
8	101	B	1082	4	-	0/7/23/23	0/3/3/3
6	MES	B	1083	-	-	0/6/14/14	0/1/1/1
10	GSP	C	1000	4	-	0/17/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1000	GSP	C8-N7	-2.08	1.30	1.34
7	A	1005	POP	P1-O	2.34	1.63	1.60
7	A	1005	POP	P2-O	2.45	1.63	1.60
10	C	1000	GSP	C6-N1	3.01	1.38	1.33
6	A	1003	MES	C5-N4	3.44	1.56	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1000	GSP	C5-C6-N1	-8.23	111.77	123.47
10	C	1000	GSP	C2-N3-C4	-2.98	111.67	115.16
10	C	1000	GSP	N3-C2-N1	-2.40	123.89	127.41
8	B	1082	101	O2P-P-O1P	2.22	119.27	110.60
10	C	1000	GSP	C6-N1-C2	6.37	125.22	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	FOK	7	0
6	A	1003	MES	1	0
8	B	1082	101	1	0
6	B	1083	MES	3	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 [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	A	189/225 (84%)	0.14	7 (3%) 41 44	32, 58, 82, 97	0
2	B	190/212 (89%)	0.09	9 (4%) 31 34	27, 42, 75, 97	0
3	C	329/394 (83%)	-0.11	8 (2%) 59 62	27, 47, 75, 98	1 (0%)
All	All	708/831 (85%)	0.01	24 (3%) 45 48	27, 48, 80, 98	1 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	MET	4.5
2	B	952	ALA	4.5
2	B	878	TYR	4.3
2	B	953	ILE	4.2
3	C	39	ALA	4.1

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. 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(\AA^2)	Q<0.9
6	MES	B	1083	12/12	0.65	0.45	90,93,99,99	4
6	MES	A	1003	12/12	0.93	0.16	72,75,80,81	0
4	MG	C	396	1/1	0.93	0.05	42,42,42,42	0
5	FOK	A	1002	29/29	0.95	0.23	33,39,46,53	0
8	101	B	1082	22/22	0.96	0.20	36,45,57,58	0
4	MG	A	581	1/1	0.97	0.07	46,46,46,46	0
10	GSP	C	1000	32/32	0.98	0.14	28,34,49,56	0
7	POP	A	1005	9/9	0.98	0.14	54,55,57,59	0
9	CL	C	398	1/1	0.99	0.19	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.