



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:15 PM GMT

PDB ID : 1SOJ
Title : CATALYTIC DOMAIN OF HUMAN PHOSPHODIESTERASE 3B IN COMPLEX WITH IBMX
Authors : Scapin, G.; Patel, S.B.; Chung, C.; Varnerin, J.P.; Edmondson, S.D.; Mastracchio, A.; Parmee, E.R.; Becker, J.W.; Singh, S.B.; Van Der Ploeg, L.H.; Tota, M.R.
Deposited on : 2004-03-15
Resolution : 2.90 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
<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

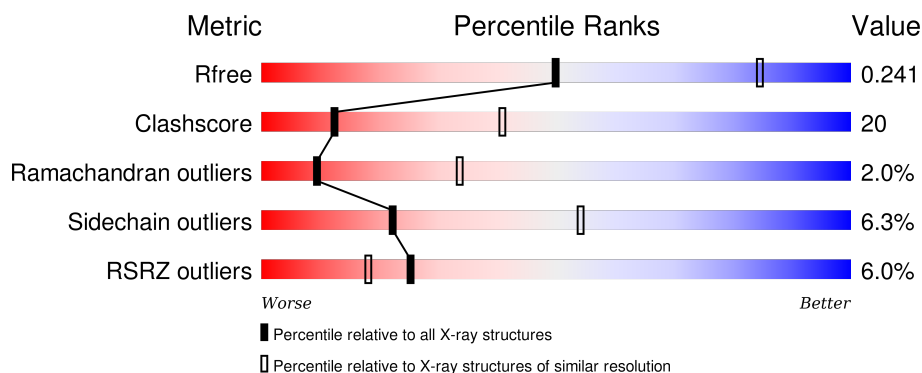
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	420	<div> <div>2%</div> <div> <div>56%</div> <div>27%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	420	<div> <div>7%</div> <div> <div>55%</div> <div>30%</div> <div>5%</div> <div>9%</div> </div> </div>
1	C	420	<div> <div>4%</div> <div> <div>55%</div> <div>29%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	420	<div> <div>6%</div> <div> <div>55%</div> <div>31%</div> <div>5%</div> <div>9%</div> </div> </div>
1	E	420	<div> <div>3%</div> <div> <div>55%</div> <div>28%</div> <div>•</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	420	<div><div></div><div>4%</div><div>58%</div><div>29%</div><div>5%</div><div>9%</div></div>
1	G	420	<div><div></div><div>4%</div><div>56%</div><div>28%</div><div>•</div><div>13%</div></div>
1	H	420	<div><div></div><div>6%</div><div>55%</div><div>31%</div><div>5%</div><div>9%</div></div>
1	I	420	<div><div></div><div>3%</div><div>58%</div><div>25%</div><div>•</div><div>13%</div></div>
1	J	420	<div><div></div><div>3%</div><div>55%</div><div>31%</div><div>5%</div><div>9%</div></div>
1	K	420	<div><div></div><div>14%</div><div>57%</div><div>27%</div><div>•</div><div>13%</div></div>
1	L	420	<div><div></div><div>9%</div><div>55%</div><div>30%</div><div>5%</div><div>9%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36048 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 cGMP-inhibited 3',5'-cyclic phosphodiesterase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	B	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	C	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	D	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	E	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	F	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	G	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	H	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	I	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	J	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	K	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	L	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

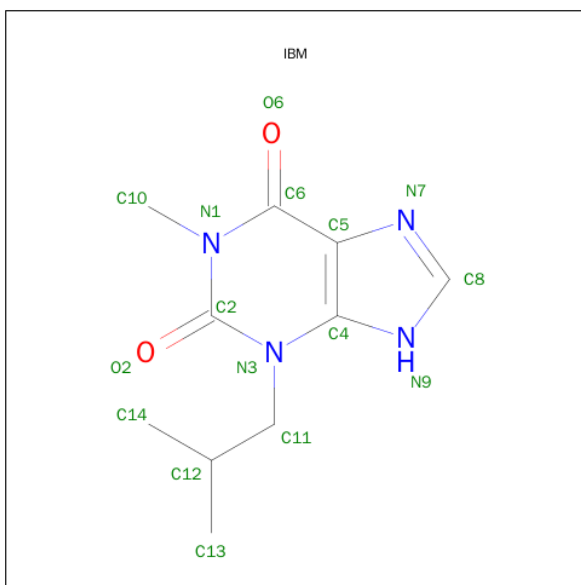
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mg	0	0
			2	2		
2	J	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mg	0	0
			2	2		
2	K	2	Total	Mg	0	0
			2	2		
2	E	2	Total	Mg	0	0
			2	2		
2	H	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	I	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	L	2	Total	Mg	0	0
			2	2		
2	F	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 3-ISOBUTYL-1-METHYLNANTHINE (three-letter code: IBM) (formula: $C_{10}H_{14}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	10	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			16	10	4	2		
3	C	1	Total	C	N	O	0	0
			16	10	4	2		
3	D	1	Total	C	N	O	0	0
			16	10	4	2		
3	E	1	Total	C	N	O	0	0
			16	10	4	2		
3	F	1	Total	C	N	O	0	0
			16	10	4	2		
3	G	1	Total	C	N	O	0	0
			16	10	4	2		
3	H	1	Total	C	N	O	0	0
			16	10	4	2		
3	I	1	Total	C	N	O	0	0
			16	10	4	2		
3	J	1	Total	C	N	O	0	0
			16	10	4	2		
3	K	1	Total	C	N	O	0	0
			16	10	4	2		
3	L	1	Total	C	N	O	0	0
			16	10	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	24	Total	O	0	0
			24	24		
4	C	24	Total	O	0	0
			24	24		
4	D	24	Total	O	0	0
			24	24		
4	E	23	Total	O	0	0
			23	23		
4	F	25	Total	O	0	0
			25	25		
4	G	23	Total	O	0	0
			23	23		
4	H	25	Total	O	0	0
			25	25		

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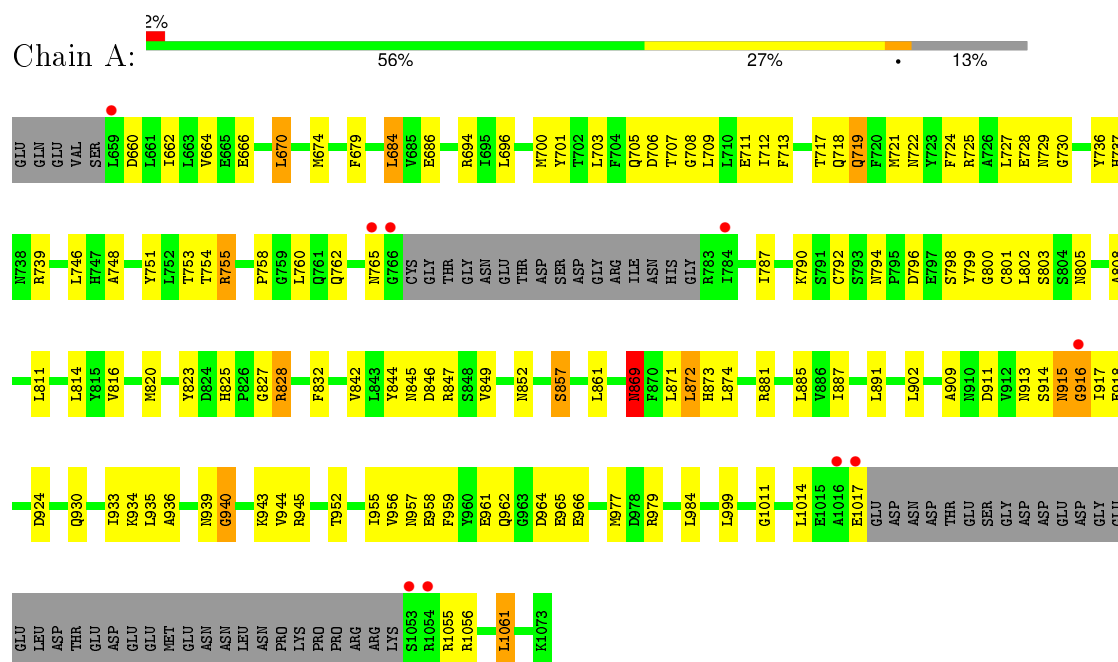
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	24	Total 24	O 24	0	0
4	J	24	Total 24	O 24	0	0
4	K	24	Total 24	O 24	0	0
4	L	24	Total 24	O 24	0	0

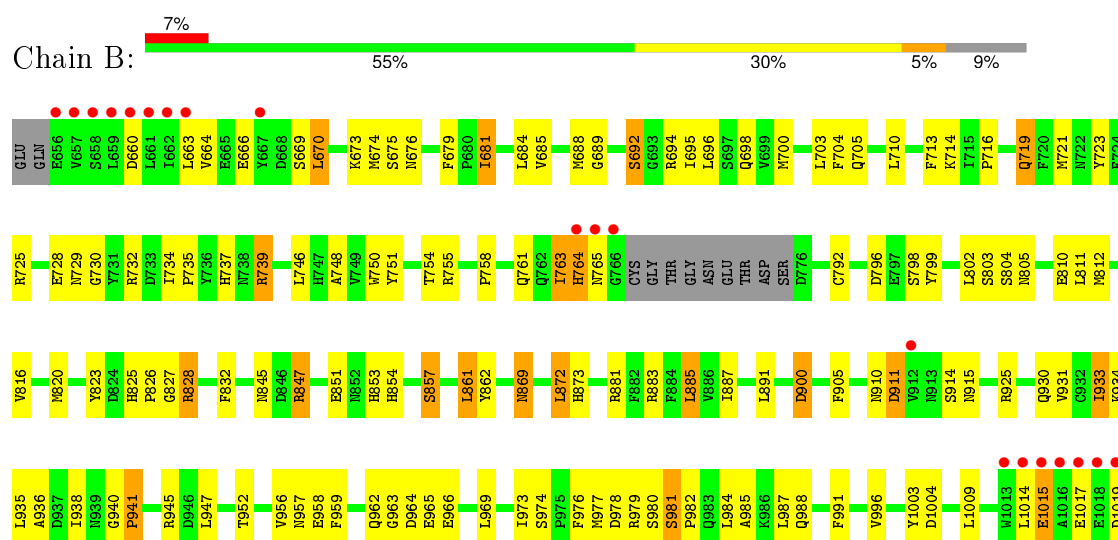
3 Residue-property plots

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.

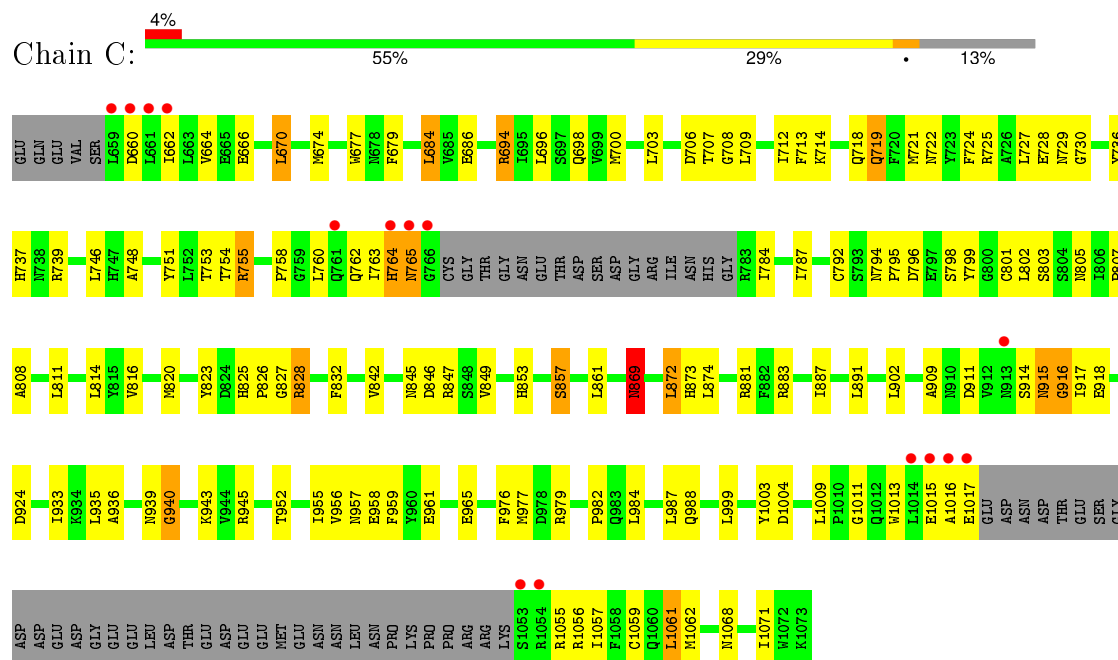
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



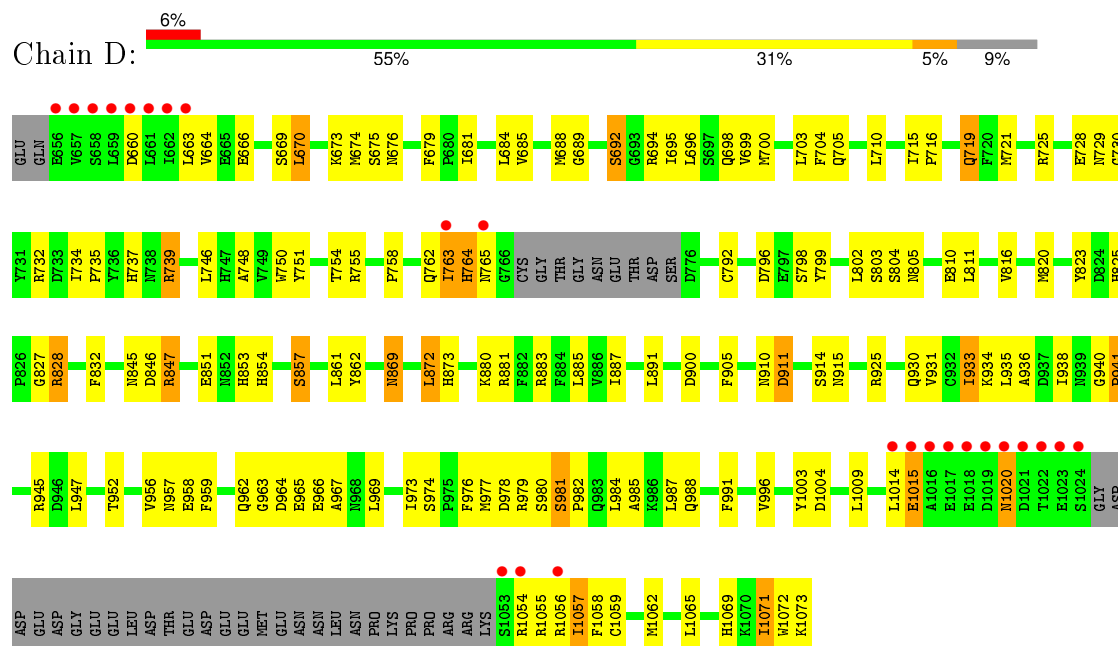
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

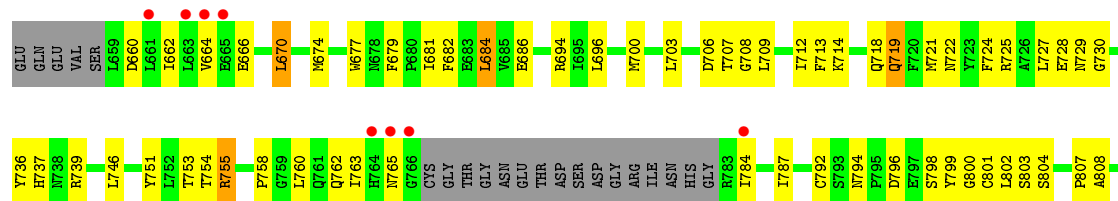
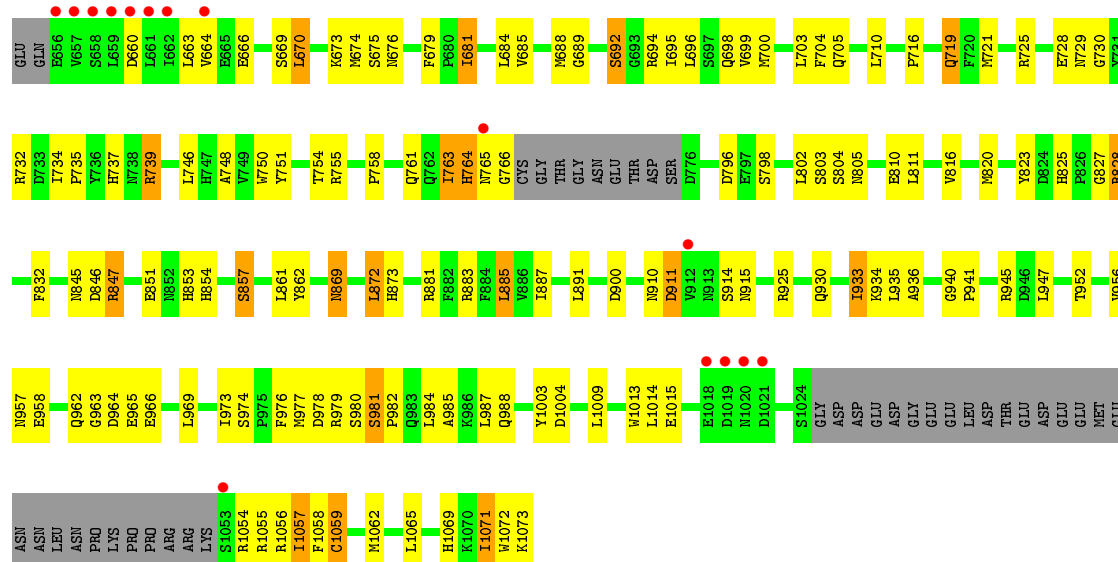
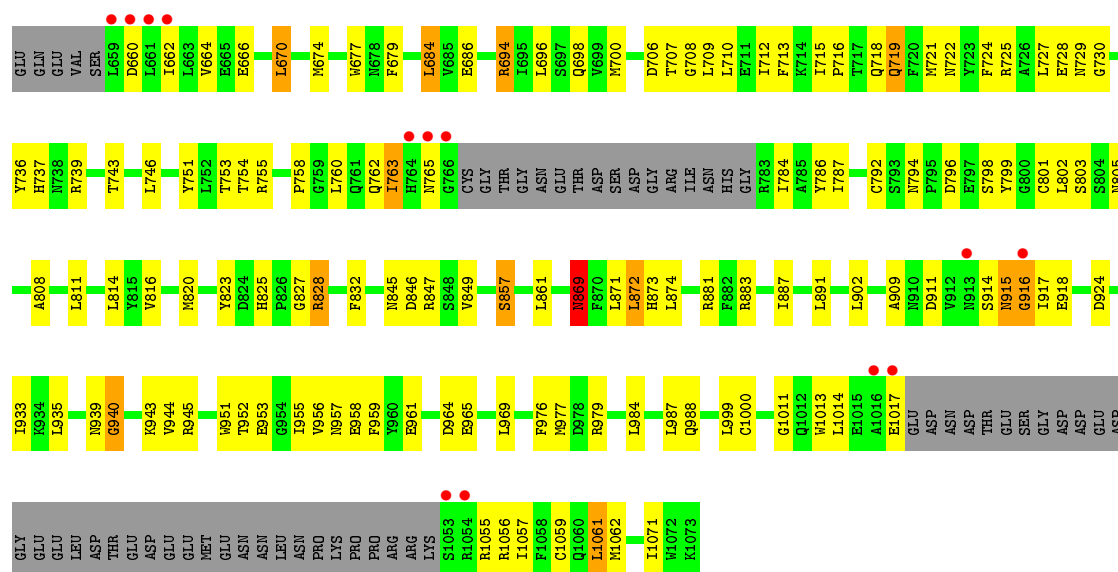


- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

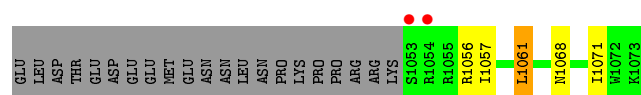


- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

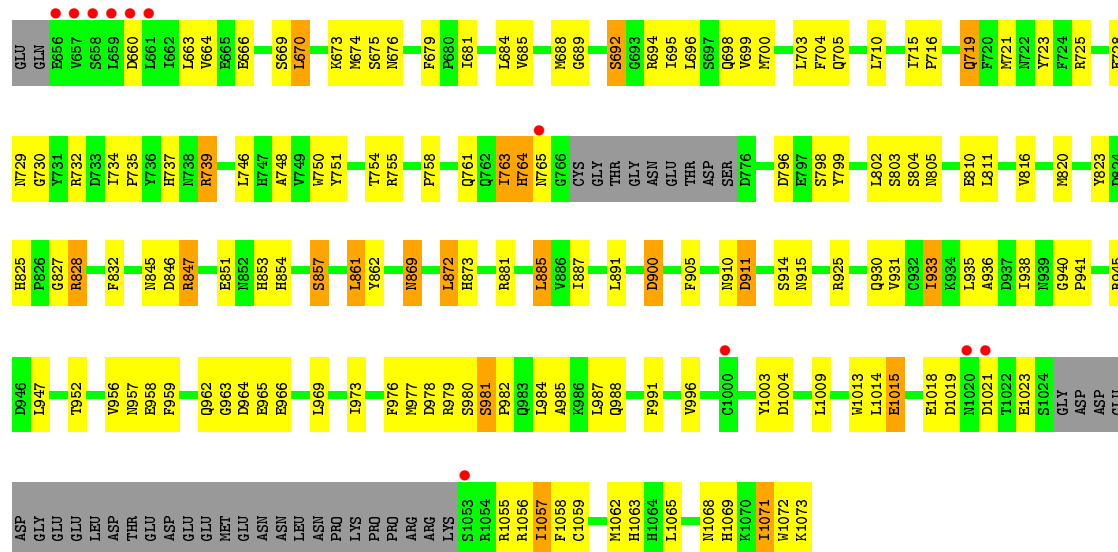




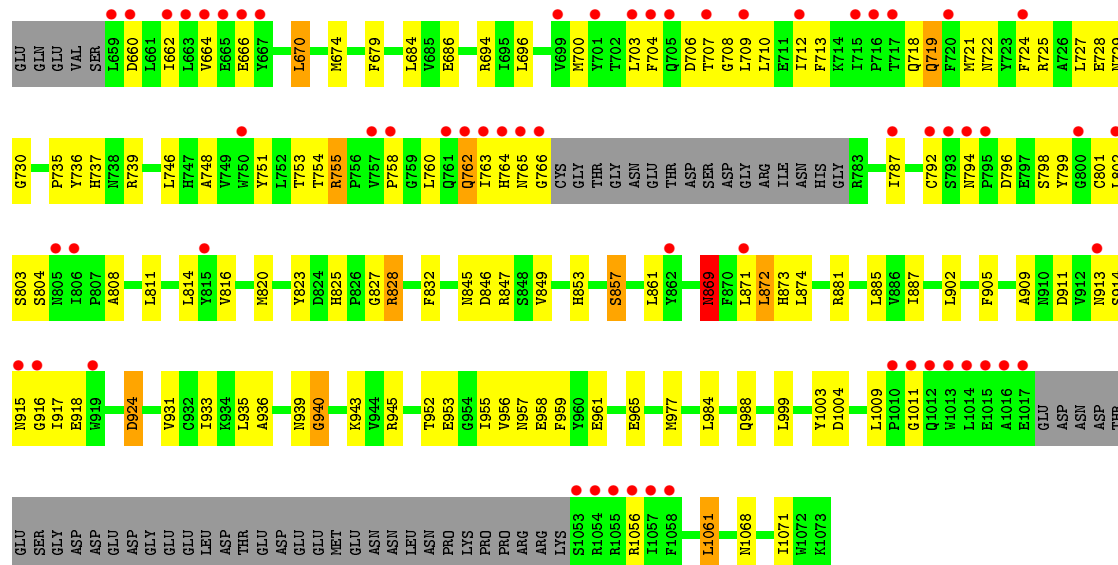




- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



GLU	GLN	N729	Y823	L935	W1013	E1014	E1015	A1016	E1017	E1018	D1019	M1020	D1021	T1022	E1023	S1024	GLY	ASP	ASP	GLU	ASP	GLU	GLY	GLU	GLU	LEU	ASP	THR	GLU	ASP	GLU	GLY	GLU	ASN	ASN	LEU	ASN	PRO	LYS	PRO	ARG	ARG	LYS	S1053	R1054	R1055	R1056	T1057	F1058	C1059	M1062	H1063	H1064	L1065	M1068	H1069	K1070	T1071	W1072	K1073																																					
		G730	H824	D936	E937	I938	N939	G940	P941	A942	K943	V944	R945	D946	L947	E948	T952	V956	N957	E958	F959	Q962	G963	D964	E965	E966	A967	N968	L969	G970	L971	F972	I973	S974	P975	V976	N977	D978	R979	S980	P982	Q983	L984	A985	K986	L987	Q988	F991	V996	Y1003	D1004	L1009	Q1012																																												
		Y731	H825	D937	I938	N939	G940	P941	A942	K943	V944	R945	D946	L947	E948	T952	V956	N957	E958	F959	Q962	G963	D964	E965	E966	A967	N968	L969	G970	L971	F972	I973	S974	P975	V976	N977	D978	R979	S980	P982	Q983	L984	A985	K986	L987	Q988	F991	V996	Y1003	D1004	L1009	Q1012																																													
		R732	H826	D938	I939	N940	G941	P942	A943	K944	V945	R946	D947	E949	T953	V957	N958	E959	F960	Q963	G964	D965	E966	A968	N969	L970	G971	L972	F973	I974	S975	P976	V977	N978	D979	R980	S981	T982	Q984	R985	L986	A987	K987	L988	Q989	F992	V997	Y1004	D1005	L1010	Q1013																																														
E856	V857	S858	L859	D860	L861	I862	L863	V864	E865	E866	S869	L870	K873	M874	S875	N876	F879	P880	I881	L884	V885	M888	G889	S892	G893	R894	I895	L896	S897	Q898	V899	M700	L703	F704	Q705	L710	I715	P716	Q719	F720	M721	N722	Y723	F724	R725	E728																																																			
																																															Y731	R732	I734	P735	Y736	H737	N738	R739	L746	H747	A748	Y749	W750	Y751	T754	R755	P758	G759	L760	Q761	Q762	H763	H764	N765	G766	CYS	GLY	THR	GLY	ASN	GLU	THR	ASP	SER	D776	N794	P795	D796	E797	S798	Y799	L802	S803	S804	N805	E810	L811	W816	M820		
																																															Y823	H824	D937	I938	N939	G940	P941	A942	K943	V944	R945	D946	L947	E948	T952	V956	N957	E958	F959	Q962	G963	D964	E965	E966	A967	N968	L969	G970	L971	F972	I973	S974	P975	V976	N977	D978	R979	S980	P982	Q983	L984	A985	K986	L987	Q988	F991	V996	Y1003	D1004	L1009	Q1012
																																															Y823	H824	D937	I938	N939	G940	P941	A942	K943	V944	R945	D946	L947	E948	T952	V956	N957	E958	F959	Q962	G963	D964	E965	E966	A967	N968	L969	G970	L971	F972	I973	S974	P975	V976	N977	D978	R979	S980	P982	Q983	L984	A985	K986	L987	Q988	F991	V996	Y1003	D1004	L1009	Q1012

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	275.05Å 147.08Å 253.49Å 90.00° 109.84° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 49.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.90) 96.6 (49.61-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.91Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.231 , 0.249 0.227 , 0.241	Depositor DCC
R_{free} test set	10121 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 203261 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	36048	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: MG, IBM

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	0.45	0/2982	0.59	0/4053
1	B	0.44	0/3092	0.59	0/4203
1	C	0.45	0/2982	0.59	0/4053
1	D	0.47	0/3092	0.60	0/4203
1	E	0.47	1/2982 (0.0%)	0.59	0/4053
1	F	0.46	0/3092	0.59	0/4203
1	G	0.45	0/2982	0.59	0/4053
1	H	0.45	0/3092	0.59	1/4203 (0.0%)
1	I	0.45	0/2982	0.58	0/4053
1	J	0.46	0/3092	0.59	0/4203
1	K	0.47	0/2982	0.59	0/4053
1	L	0.47	0/3092	0.60	0/4203
All	All	0.46	1/36444 (0.0%)	0.59	1/49536 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1000	CYS	CB-SG	-5.15	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	795	PRO	N-CA-CB	5.03	109.34	103.30

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	2907	0	2772	110	0
1	B	3017	0	2834	132	0
1	C	2907	0	2772	124	0
1	D	3017	0	2834	134	0
1	E	2907	0	2772	114	0
1	F	3017	0	2834	119	0
1	G	2907	0	2772	109	0
1	H	3017	0	2834	126	0
1	I	2907	0	2772	108	0
1	J	3017	0	2834	143	0
1	K	2907	0	2772	108	0
1	L	3017	0	2834	125	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	16	0	14	0	0
3	B	16	0	14	0	0
3	C	16	0	14	0	0
3	D	16	0	14	0	0
3	E	16	0	14	0	0
3	F	16	0	14	0	0
3	G	16	0	14	0	0
3	H	16	0	14	0	0
3	I	16	0	14	0	0
3	J	16	0	14	0	0
3	K	16	0	14	0	0
3	L	16	0	14	0	0
4	A	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	0	3	0
4	C	24	0	0	1	0
4	D	24	0	0	1	0
4	E	23	0	0	2	0
4	F	25	0	0	1	0
4	G	23	0	0	1	0
4	H	25	0	0	0	0
4	I	24	0	0	1	0
4	J	24	0	0	0	0
4	K	24	0	0	1	0
4	L	24	0	0	1	0
All	All	36048	0	33804	1360	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 20.

The worst 5 of 1360 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:E:825:HIS:HD2	1:E:827:GLY:H	1.10	1.00
1:A:719:GLN:H	1:A:719:GLN:HE21	1.04	1.00
1:I:719:GLN:HE21	1:I:719:GLN:H	1.06	0.98
1:K:762:GLN:HE22	1:K:804:SER:HB2	1.28	0.98
1:K:719:GLN:H	1:K:719:GLN:HE21	1.06	0.98

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	358/420 (85%)	332 (93%)	21 (6%)	5 (1%)	14 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	375/420 (89%)	337 (90%)	28 (8%)	10 (3%)	6	25
1	C	358/420 (85%)	330 (92%)	22 (6%)	6 (2%)	11	38
1	D	375/420 (89%)	334 (89%)	31 (8%)	10 (3%)	6	25
1	E	358/420 (85%)	334 (93%)	18 (5%)	6 (2%)	11	38
1	F	375/420 (89%)	335 (89%)	31 (8%)	9 (2%)	7	29
1	G	358/420 (85%)	333 (93%)	22 (6%)	3 (1%)	24	60
1	H	375/420 (89%)	339 (90%)	28 (8%)	8 (2%)	9	32
1	I	358/420 (85%)	332 (93%)	20 (6%)	6 (2%)	11	38
1	J	375/420 (89%)	338 (90%)	28 (8%)	9 (2%)	7	29
1	K	358/420 (85%)	327 (91%)	25 (7%)	6 (2%)	11	38
1	L	375/420 (89%)	334 (89%)	30 (8%)	11 (3%)	6	23
All	All	4398/5040 (87%)	4005 (91%)	304 (7%)	89 (2%)	9	33

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	869	ASN
1	C	765	ASN
1	C	869	ASN
1	D	764	HIS
1	E	763	ILE

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	306/370 (83%)	288 (94%)	18 (6%)	24	58
1	B	313/370 (85%)	291 (93%)	22 (7%)	19	47
1	C	306/370 (83%)	290 (95%)	16 (5%)	29	64
1	D	313/370 (85%)	291 (93%)	22 (7%)	19	47
1	E	306/370 (83%)	291 (95%)	15 (5%)	31	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	313/370 (85%)	292 (93%)	21 (7%)	20	50
1	G	306/370 (83%)	287 (94%)	19 (6%)	23	55
1	H	313/370 (85%)	291 (93%)	22 (7%)	19	47
1	I	306/370 (83%)	288 (94%)	18 (6%)	24	58
1	J	313/370 (85%)	292 (93%)	21 (7%)	20	50
1	K	306/370 (83%)	288 (94%)	18 (6%)	24	58
1	L	313/370 (85%)	292 (93%)	21 (7%)	20	50
All	All	3714/4440 (84%)	3481 (94%)	233 (6%)	22	54

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	900	ASP
1	G	965	GLU
1	L	719	GLN
1	F	933	ILE
1	G	706	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	737	HIS
1	G	913	ASN
1	K	957	ASN
1	F	825	HIS
1	G	719	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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	IBM	A	2111	-	9,17,17	3.54	3 (33%)	9,25,25	0.66	0
3	IBM	B	2112	-	9,17,17	3.12	3 (33%)	9,25,25	0.71	0
3	IBM	C	2113	-	9,17,17	3.38	3 (33%)	9,25,25	0.68	0
3	IBM	D	2114	-	9,17,17	3.30	3 (33%)	9,25,25	0.56	0
3	IBM	E	2115	-	9,17,17	3.30	3 (33%)	9,25,25	0.69	0
3	IBM	F	2116	-	9,17,17	2.98	3 (33%)	9,25,25	0.62	0
3	IBM	G	2117	-	9,17,17	3.24	3 (33%)	9,25,25	0.71	0
3	IBM	H	2118	-	9,17,17	3.16	3 (33%)	9,25,25	0.65	0
3	IBM	I	2119	-	9,17,17	3.17	3 (33%)	9,25,25	0.67	0
3	IBM	J	2120	-	9,17,17	3.18	3 (33%)	9,25,25	0.62	0
3	IBM	K	2121	-	9,17,17	3.34	3 (33%)	9,25,25	0.56	0
3	IBM	L	2122	-	9,17,17	3.31	3 (33%)	9,25,25	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IBM	A	2111	-	-	0/4/4/4	0/2/2/2
3	IBM	B	2112	-	-	0/4/4/4	0/2/2/2
3	IBM	C	2113	-	-	0/4/4/4	0/2/2/2
3	IBM	D	2114	-	-	0/4/4/4	0/2/2/2
3	IBM	E	2115	-	-	0/4/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IBM	F	2116	-	-	0/4/4/4	0/2/2/2
3	IBM	G	2117	-	-	0/4/4/4	0/2/2/2
3	IBM	H	2118	-	-	0/4/4/4	0/2/2/2
3	IBM	I	2119	-	-	0/4/4/4	0/2/2/2
3	IBM	J	2120	-	-	0/4/4/4	0/2/2/2
3	IBM	K	2121	-	-	0/4/4/4	0/2/2/2
3	IBM	L	2122	-	-	0/4/4/4	0/2/2/2

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2113	IBM	C5-C4	-3.18	1.33	1.40
3	A	2111	IBM	C5-C4	-3.18	1.33	1.40
3	J	2120	IBM	C5-C4	-3.07	1.33	1.40
3	B	2112	IBM	C5-C4	-3.04	1.33	1.40
3	I	2119	IBM	C5-C4	-3.02	1.33	1.40

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	364/420 (86%)	0.01	9 (2%) 61 55	24, 42, 80, 100	0
1	B	381/420 (90%)	0.35	29 (7%) 17 11	25, 50, 92, 100	0
1	C	364/420 (86%)	0.10	15 (4%) 41 34	26, 43, 81, 100	0
1	D	381/420 (90%)	0.36	24 (6%) 23 17	22, 47, 89, 100	0
1	E	364/420 (86%)	0.08	13 (3%) 46 38	23, 42, 81, 100	0
1	F	381/420 (90%)	0.16	15 (3%) 43 36	21, 45, 79, 100	0
1	G	364/420 (86%)	-0.01	15 (4%) 41 34	24, 44, 83, 100	0
1	H	381/420 (90%)	0.30	24 (6%) 23 17	29, 52, 92, 100	0
1	I	364/420 (86%)	0.08	14 (3%) 44 37	23, 42, 81, 100	0
1	J	381/420 (90%)	0.12	11 (2%) 55 49	22, 46, 77, 100	0
1	K	364/420 (86%)	0.66	60 (16%) 2 1	28, 51, 87, 100	0
1	L	381/420 (90%)	0.57	39 (10%) 9 5	29, 54, 91, 100	0
All	All	4470/5040 (88%)	0.23	268 (5%) 25 18	21, 46, 85, 100	0

The worst 5 of 268 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	659	LEU	11.9
1	H	1022	THR	11.7
1	B	1024	SER	11.6
1	D	1021	ASP	10.9
1	H	1020	ASN	10.7

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

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

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
3	IBM	G	2117	16/16	0.96	0.21	1.56	44,49,50,51	0
3	IBM	C	2113	16/16	0.98	0.19	1.18	36,42,48,48	0
3	IBM	H	2118	16/16	0.93	0.25	1.05	72,78,79,80	0
3	IBM	B	2112	16/16	0.95	0.24	0.94	54,56,59,59	0
3	IBM	K	2121	16/16	0.97	0.19	0.78	54,59,60,61	0
3	IBM	J	2120	16/16	0.98	0.23	0.69	31,35,40,41	0
3	IBM	E	2115	16/16	0.97	0.19	0.63	28,32,35,37	0
3	IBM	I	2119	16/16	0.98	0.19	0.48	35,38,39,39	0
3	IBM	D	2114	16/16	0.96	0.20	0.18	35,53,56,57	0
3	IBM	A	2111	16/16	0.97	0.18	0.06	36,38,42,42	0
3	IBM	L	2122	16/16	0.94	0.22	0.03	68,77,78,79	0
2	MG	H	2137	1/1	0.97	0.13	-0.45	12,12,12,12	0
2	MG	C	2127	1/1	1.00	0.14	-0.49	5,5,5,5	0
2	MG	F	2133	1/1	0.99	0.15	-0.69	1,1,1,1	0
2	MG	L	2145	1/1	0.98	0.12	-0.85	23,23,23,23	0
2	MG	D	2129	1/1	0.99	0.16	-0.90	9,9,9,9	0
2	MG	K	2143	1/1	0.98	0.12	-0.94	20,20,20,20	0
2	MG	I	2139	1/1	0.99	0.15	-1.06	5,5,5,5	0
2	MG	J	2141	1/1	0.99	0.14	-1.28	6,6,6,6	0
2	MG	K	2144	1/1	0.99	0.12	-1.30	40,40,40,40	0
3	IBM	F	2116	16/16	0.98	0.17	-1.30	28,37,40,40	0
2	MG	E	2131	1/1	0.99	0.15	-1.32	1,1,1,1	0
2	MG	A	2123	1/1	0.99	0.13	-1.43	2,2,2,2	0
2	MG	G	2135	1/1	0.99	0.12	-1.73	1,1,1,1	0
2	MG	B	2125	1/1	0.98	0.10	-2.40	4,4,4,4	0
2	MG	E	2132	1/1	0.99	0.14	-2.50	29,29,29,29	0
2	MG	B	2126	1/1	0.93	0.11	-2.55	56,56,56,56	0
2	MG	A	2124	1/1	0.99	0.11	-2.69	41,41,41,41	0
2	MG	C	2128	1/1	0.99	0.10	-2.72	29,29,29,29	0
2	MG	I	2140	1/1	0.95	0.12	-2.94	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	J	2142	1/1	0.99	0.11	-3.03	39,39,39,39	0
2	MG	L	2146	1/1	0.97	0.07	-3.08	30,30,30,30	0
2	MG	G	2136	1/1	0.99	0.10	-3.30	28,28,28,28	0
2	MG	D	2130	1/1	0.99	0.11	-3.36	22,22,22,22	0
2	MG	H	2138	1/1	0.97	0.06	-3.96	32,32,32,32	0
2	MG	F	2134	1/1	0.98	0.07	-4.94	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.