



wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 01:41 AM 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 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/ValidationPDFNotes.html>

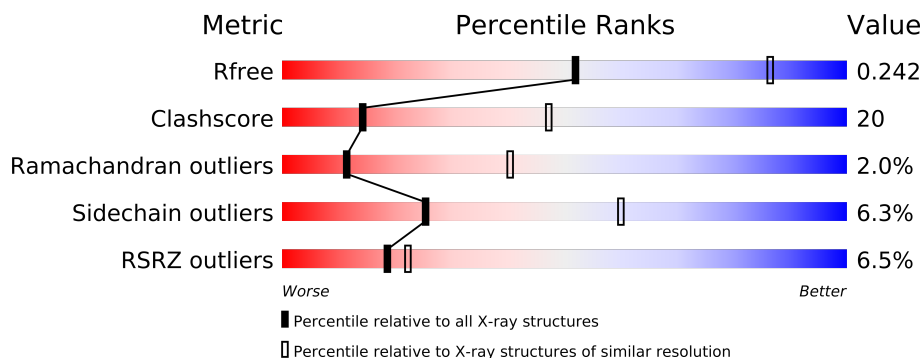
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	420	
1	B	420	
1	C	420	
1	D	420	
1	E	420	
1	F	420	
1	G	420	
1	H	420	
1	I	420	
1	J	420	
1	K	420	
1	L	420	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36048 atoms, of which 0 are hydrogen and 0 are deuterium.

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).

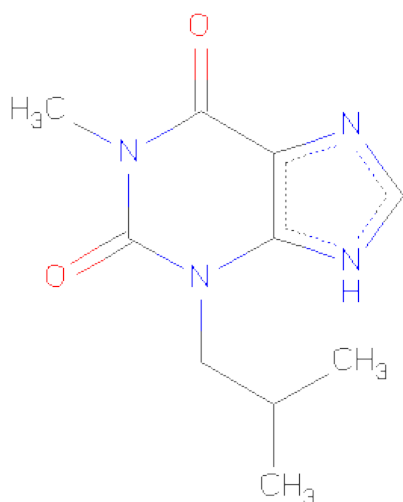
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mg	0	0
			2	2		
2	J	2	Total	Mg	0	0
			2	2		

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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-METHYLBXANTHINE (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		

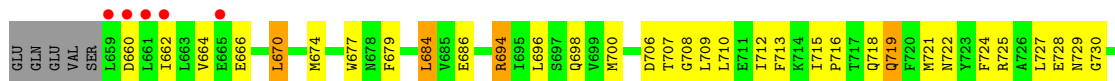
- Molecule 4 is water.

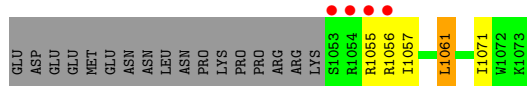
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	24	Total	O	0	0
			24	24		
4	C	24	Total	O	0	0
			24	24		
4	D	24	Total	O	0	0
			24	24		
4	E	23	Total	O	0	0
			23	23		
4	F	25	Total	O	0	0
			25	25		
4	G	23	Total	O	0	0
			23	23		
4	H	25	Total	O	0	0
			25	25		

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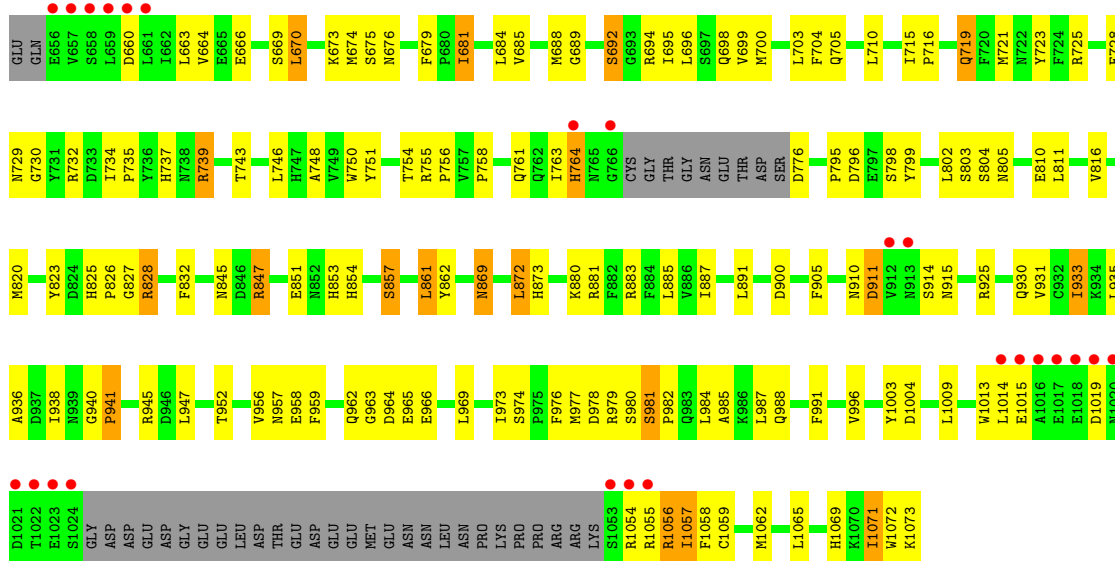
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	24	Total 24	O 24	0	0
4	J	24	Total 24	O 24	0	0
4	K	24	Total 24	O 24	0	0
4	L	24	Total 24	O 24	0	0





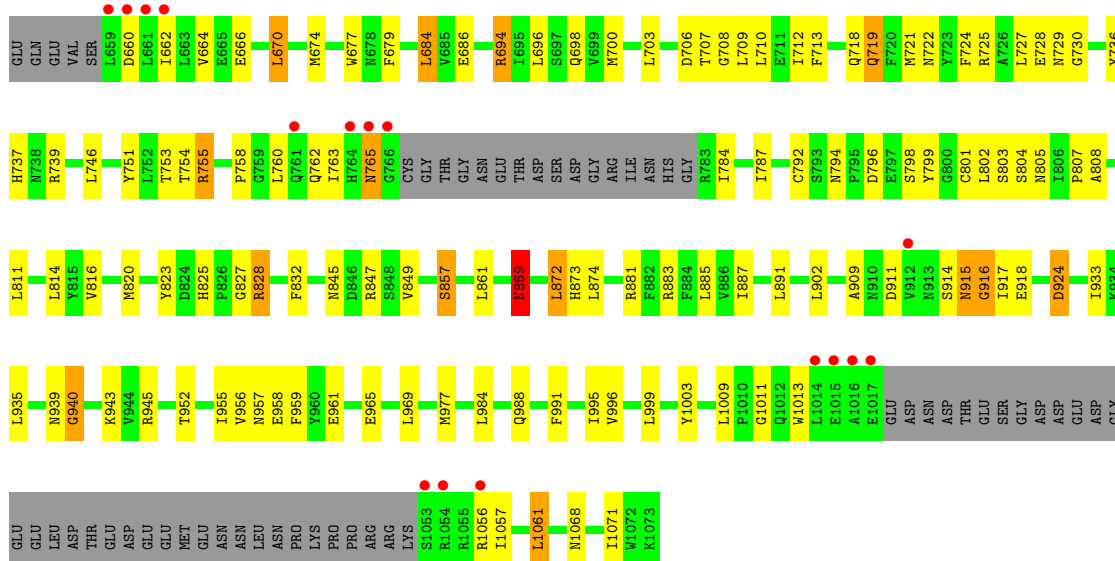
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

Chain H:



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

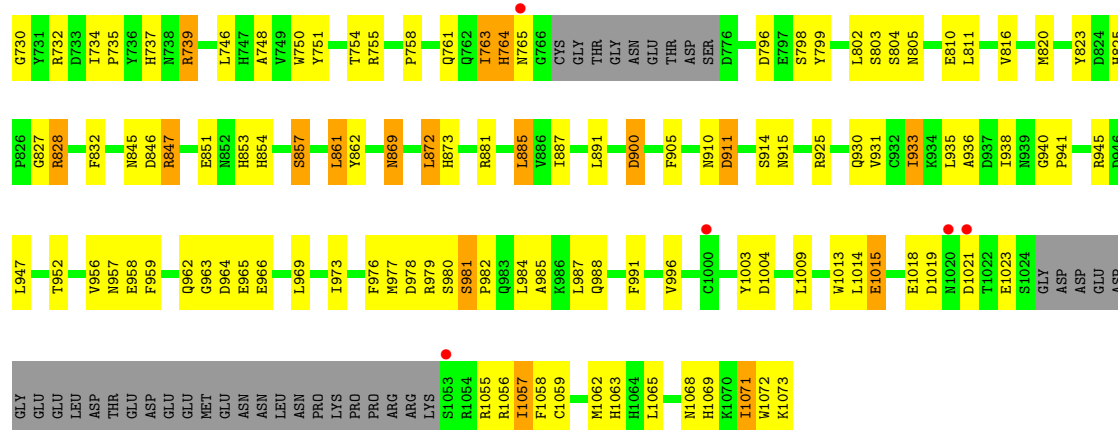
Chain I:



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

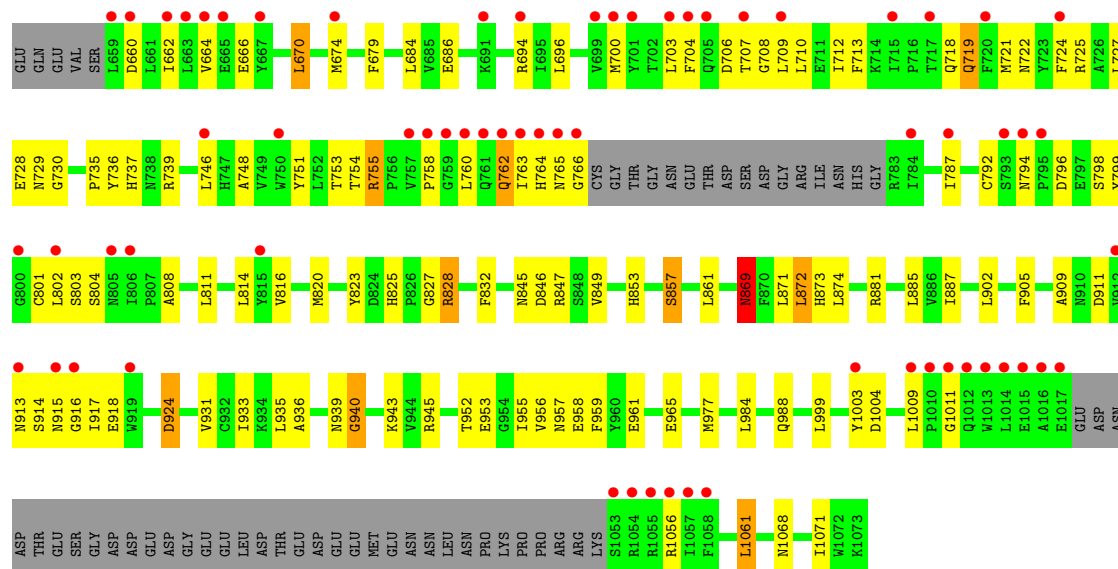
Chain J:





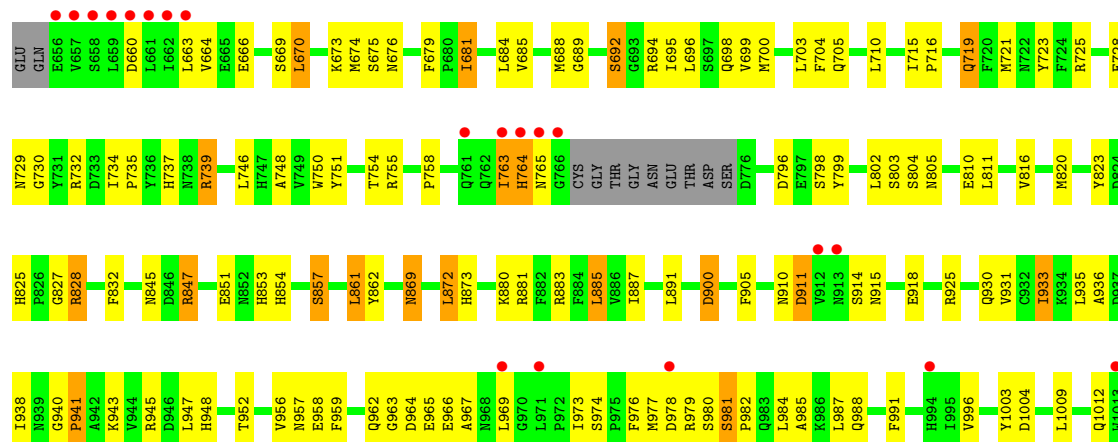
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

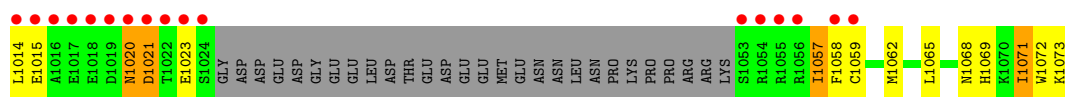
Chain K:



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

Chain L:





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 0.228 , 0.242	Depositor DCC
R_{free} test set	10128 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)	0.33 , 24.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	16	0	14	0	0
4	A	24	0	0	1	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

The worst 5 of 1360 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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%)	16 52
1	B	375/420 (89%)	337 (90%)	28 (8%)	10 (3%)	8 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	358/420 (85%)	330 (92%)	22 (6%)	6 (2%)	14 45
1	D	375/420 (89%)	334 (89%)	31 (8%)	10 (3%)	8 30
1	E	358/420 (85%)	334 (93%)	18 (5%)	6 (2%)	14 45
1	F	375/420 (89%)	335 (89%)	31 (8%)	9 (2%)	9 35
1	G	358/420 (85%)	333 (93%)	22 (6%)	3 (1%)	27 68
1	H	375/420 (89%)	339 (90%)	28 (8%)	8 (2%)	11 39
1	I	358/420 (85%)	332 (93%)	20 (6%)	6 (2%)	14 45
1	J	375/420 (89%)	338 (90%)	28 (8%)	9 (2%)	9 35
1	K	358/420 (85%)	327 (91%)	25 (7%)	6 (2%)	14 45
1	L	375/420 (89%)	334 (89%)	30 (8%)	11 (3%)	7 28
All	All	4398/5040 (87%)	4005 (91%)	304 (7%)	89 (2%)	11 40

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%)	28 64
1	B	313/370 (85%)	291 (93%)	22 (7%)	21 53
1	C	306/370 (83%)	290 (95%)	16 (5%)	32 71
1	D	313/370 (85%)	291 (93%)	22 (7%)	21 53
1	E	306/370 (83%)	291 (95%)	15 (5%)	35 73
1	F	313/370 (85%)	292 (93%)	21 (7%)	23 56
1	G	306/370 (83%)	287 (94%)	19 (6%)	26 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	313/370 (85%)	291 (93%)	22 (7%)	21	53
1	I	306/370 (83%)	288 (94%)	18 (6%)	28	64
1	J	313/370 (85%)	292 (93%)	21 (7%)	23	56
1	K	306/370 (83%)	288 (94%)	18 (6%)	28	64
1	L	313/370 (85%)	292 (93%)	21 (7%)	23	56
All	All	3714/4440 (84%)	3481 (94%)	233 (6%)	25	60

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 chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	-	17,17,17	2.18	5 (29%)	20,25,25	13.27	5 (25%)
3	IBM	B	2112	-	17,17,17	2.12	5 (29%)	20,25,25	15.12	5 (25%)
3	IBM	C	2113	-	17,17,17	2.21	5 (29%)	20,25,25	11.21	5 (25%)
3	IBM	D	2114	-	17,17,17	2.37	7 (41%)	20,25,25	12.36	6 (30%)
3	IBM	E	2115	-	17,17,17	2.10	6 (35%)	20,25,25	14.16	5 (25%)
3	IBM	F	2116	-	17,17,17	2.00	4 (23%)	20,25,25	13.59	5 (25%)
3	IBM	G	2117	-	17,17,17	2.16	5 (29%)	20,25,25	11.95	5 (25%)
3	IBM	H	2118	-	17,17,17	2.24	6 (35%)	20,25,25	12.79	5 (25%)
3	IBM	I	2119	-	17,17,17	2.19	5 (29%)	20,25,25	11.59	4 (20%)
3	IBM	J	2120	-	17,17,17	2.19	6 (35%)	20,25,25	13.10	5 (25%)
3	IBM	K	2121	-	17,17,17	2.22	6 (35%)	20,25,25	14.60	5 (25%)
3	IBM	L	2122	-	17,17,17	2.28	6 (35%)	20,25,25	14.20	6 (30%)

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	0/0/2/2
3	IBM	B	2112	-	-	0/4/4/4	0/0/2/2
3	IBM	C	2113	-	-	0/4/4/4	0/0/2/2
3	IBM	D	2114	-	-	0/4/4/4	0/0/2/2
3	IBM	E	2115	-	-	0/4/4/4	0/0/2/2
3	IBM	F	2116	-	-	0/4/4/4	0/0/2/2
3	IBM	G	2117	-	-	0/4/4/4	0/0/2/2
3	IBM	H	2118	-	-	0/4/4/4	0/0/2/2
3	IBM	I	2119	-	-	0/4/4/4	0/0/2/2
3	IBM	J	2120	-	-	0/4/4/4	0/0/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IBM	K	2121	-	-	0/4/4/4	0/0/2/2
3	IBM	L	2122	-	-	0/4/4/4	0/0/2/2

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2113	IBM	C6-C5	5.51	1.50	1.41
3	D	2114	IBM	C6-C5	5.49	1.50	1.41
3	J	2120	IBM	C6-C5	5.48	1.50	1.41
3	G	2117	IBM	C6-C5	5.37	1.50	1.41
3	I	2119	IBM	C6-C5	5.33	1.49	1.41

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2112	IBM	C6-C5-N7	-66.31	130.71	134.24
3	K	2121	IBM	C6-C5-N7	-63.55	130.86	134.24
3	L	2122	IBM	C6-C5-N7	-61.99	130.94	134.24
3	E	2115	IBM	C6-C5-N7	-61.50	130.97	134.24
3	F	2116	IBM	C6-C5-N7	-59.17	131.09	134.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.04	11 (3%) 48 57	24, 42, 80, 100	0
1	B	381/420 (90%)	0.37	30 (7%) 13 15	25, 50, 92, 100	0
1	C	364/420 (86%)	0.16	18 (4%) 28 34	26, 43, 81, 100	0
1	D	381/420 (90%)	0.40	29 (7%) 14 17	22, 47, 89, 100	0
1	E	364/420 (86%)	0.12	15 (4%) 35 43	23, 42, 81, 100	0
1	F	381/420 (90%)	0.19	16 (4%) 35 41	21, 45, 79, 100	0
1	G	364/420 (86%)	0.05	19 (5%) 26 32	24, 44, 83, 100	0
1	H	381/420 (90%)	0.30	24 (6%) 19 23	29, 52, 92, 100	0
1	I	364/420 (86%)	0.12	16 (4%) 33 40	23, 42, 81, 100	0
1	J	381/420 (90%)	0.14	10 (2%) 53 63	22, 46, 77, 100	0
1	K	364/420 (86%)	0.68	65 (17%) 2 3	28, 51, 87, 100	0
1	L	381/420 (90%)	0.57	37 (9%) 8 10	29, 54, 91, 100	0
All	All	4470/5040 (88%)	0.26	290 (6%) 18 22	21, 46, 85, 100	0

The worst 5 of 290 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	659	LEU	13.0
1	B	1053	SER	11.7
1	H	1022	THR	11.4
1	C	1016	ALA	11.3
1	B	1024	SER	11.2

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	IBM	G	2117	16/16	0.22	1.78	44,49,50,51	0
3	IBM	H	2118	16/16	0.28	1.59	72,78,79,80	0
3	IBM	E	2115	16/16	0.19	1.32	28,32,35,37	0
3	IBM	B	2112	16/16	0.25	1.22	54,56,59,59	0
3	IBM	C	2113	16/16	0.18	0.94	36,42,48,48	0
3	IBM	K	2121	16/16	0.18	0.68	54,59,60,61	0
3	IBM	J	2120	16/16	0.23	0.59	31,35,40,41	0
3	IBM	D	2114	16/16	0.21	0.56	35,53,56,57	0
3	IBM	A	2111	16/16	0.19	0.52	36,38,42,42	0
3	IBM	I	2119	16/16	0.19	0.38	35,38,39,39	0
3	IBM	L	2122	16/16	0.23	0.26	68,77,78,79	0
2	MG	C	2127	1/1	0.15	0.12	5,5,5,5	0
2	MG	H	2137	1/1	0.13	-0.10	12,12,12,12	0
2	MG	I	2139	1/1	0.15	-0.49	5,5,5,5	0
2	MG	L	2145	1/1	0.13	-0.49	23,23,23,23	0
2	MG	F	2133	1/1	0.15	-0.57	1,1,1,1	0
2	MG	D	2129	1/1	0.15	-0.72	9,9,9,9	0
2	MG	K	2143	1/1	0.12	-0.84	20,20,20,20	0
3	IBM	F	2116	16/16	0.17	-0.99	28,37,40,40	0
2	MG	K	2144	1/1	0.13	-1.00	40,40,40,40	0
2	MG	J	2141	1/1	0.14	-1.24	6,6,6,6	0
2	MG	E	2131	1/1	0.15	-1.31	1,1,1,1	0
2	MG	G	2135	1/1	0.12	-1.68	1,1,1,1	0
2	MG	C	2128	1/1	0.11	-1.88	29,29,29,29	0
2	MG	A	2123	1/1	0.12	-1.89	2,2,2,2	0
2	MG	B	2126	1/1	0.11	-2.11	56,56,56,56	0
2	MG	E	2132	1/1	0.14	-2.15	29,29,29,29	0
2	MG	B	2125	1/1	0.09	-2.26	4,4,4,4	0
2	MG	J	2142	1/1	0.13	-2.39	39,39,39,39	0
2	MG	A	2124	1/1	0.11	-2.47	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	I	2140	1/1	0.13	-2.51	27,27,27,27	0
2	MG	G	2136	1/1	0.11	-2.65	28,28,28,28	0
2	MG	L	2146	1/1	0.07	-3.03	30,30,30,30	0
2	MG	D	2130	1/1	0.11	-3.07	22,22,22,22	0
2	MG	H	2138	1/1	0.06	-3.29	32,32,32,32	0
2	MG	F	2134	1/1	0.06	-5.05	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.